Sediment Transport and Metals Modeling in an Urban Stream – The Don River, Toronto

by

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AUTHOR'S DECLARATION

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

The Don River watershed has been subjected to rapid urbanization over the last few decades. As a result, vast area of built-up land has shifted the watershed’s hydrologic cycle towards lower infiltration and higher runoff rates. Such a drastic hydrologic change has resulted in frequent flooding, channel widening and erosion, and poor water quality in the region. Metals sourced from roads, landfills, industrial effluents, and wastewater treatment plant are a particularly damaging component to the system and need to be quantified and addressed. A research study was conducted by (Louie, 2014) to quantify the trace metals distribution in the Don River system and study the spatial and temporal trends of copper, lead, and zinc concentrations. It recognized the limitations in quantifying such information on a watershed scale. Efforts have been made to restore the natural water cycle of the watershed by the local authorities such as the Toronto and Region Conservation Authority (TRCA). Regional Watershed Monitoring Program (RWMP) was launched by TRCA in 2002 to monitor the surface water quality in the region. Moreover, Wet Weather Flow Management Guidelines (WWFMG) (City of Toronto, 2006) is a document currently used to design stormwater management solutions and restoration plans to control the surface water quantity and quality in the region. Challenges related to quantification of sediments and associated metals flushing through the system can be addressed through implementing appropriate modeling tools. Hydrologic models are commonly used, but they lack the capability to model instream processes that are important in case of metals. Metals can bind to the sediments and can remain in the system for years creating ‘hot spots’ of deposition with possibly elevated local levels of other pollutants. Incorporating the simulation of instream processes can enable understanding of temporal and spatial distribution of sediments and metals in detail, which is required for advanced infrastructure planning and informed decision making to restore the river network where possible and mitigate the damage where it is not.

The research aims to advance this understanding through the help of a 1-dimensional (1D) numerical model of the lower Don River extending from Taylor Creek South to the mouth of the river at Keating Channel. Total length of this reach is 9.81Km and it is confluent with two primary tributaries of the Don River, the East Don and the West Don. The metals which are focused in this study are copper, lead, and zinc as they are primarily sourced from urban centers. Hydrologic model and a hydraulic model are used in this thesis. A program is developed as a secondary objective of this thesis to link the urban hydrologic model of the river to the hydraulic model to efficiently set up the latter for detailed modeling of instream processes.

Two commercially available modeling packages are linked in this thesis. The first model is an urban watershed modeling tool called PCSWMM. TRCA has developed a hydrologic model of the entire Don River watershed using this program. Their calibrated model currently simulates the hydrology for a time span of 40 days from June 20 to July 30, 2008. The model provided by the TRCA is extended to a longer period in this thesis, and the modules for sediment and metals buildup and wash-off are activated and parameterized to simulate input loads to the channel. A second model called the Environmental Fluid Dynamics Code (EFDC) is used for advanced hydrodynamic, sediment transport, and metals fate and transport modeling of the lower Don River. The EFDC model is necessary because PCSWMM does not have the capability to simulate instream physical processes related to sediment and metals transport. Examples of processes that can be simulated in EFDC that are not possible in PCSWMM include erosion, deposition, and resuspension of sediments along with diffusion and sorption of metals to sediments. PCSWMM cannot simulate sediment bed dynamics and its pollutant composition. It only has the capability to estimate pollutant loads from subcatchments using buildup and wash-off models and land use information. It routs these loads through the hydraulic network using a completely mixed or plug flow assumption. Therefore, a dedicated model that can simulate the governing physical processes in an integrated manner is required. EFDC Explorer is used to develop a representative 1D hydrodynamic, sediment transport, and metals transport model in a coupled approach. EFDC Explorer is the commercially available user interface for pre and post processing of the EFDC model. The existing PCSWMM model of the Don River was upgraded and verified to provide pollutant loads from subcatchments spanning the time period of interest from May to August 2010.

The linking of the PCSWMM and EFDC model is achieved through development of a program written in MATLAB® R2014b. This program, called the SWMM to EFDC Model Setup tool (STEMS), creates the grid and boundary condition files in a format compatible with EFDC and reports other information for efficient setup of the EFDC model. It can be applied to any river network modelled in PCSWMM for further analysis in EFDC.

The comparison between the results of EFDC and PCSWMM model showed that the EFDC model better predicted measured suspended sediment and metals loads in comparison to the PCSWMM model alone. The hydraulic results of the two models were similar and showed high correlation. This suggested high sensitivity of EFDC hydraulic results to the boundary conditions provided by PCSWMM. However, the sediment and metal results were clearly different for the two models. The superior performance of the EFDC model further highlighted the importance of instream physical processes in sediment and contaminant transport rather than adopting simplifying assumptions. The relation of suspended sediment and total metal concentrations with river discharge suggested good agreement with the observed data set at the Todmorden monitoring station provided by TRCA and Environment Canada. Baseflow levels suggested that metals are deposited during low flow periods along with sediments and this material is resuspended during high flow events. Moreover, resulting sediment bed metal concentrations at the mouth of the river also agreed with the suggested trend provided by TRCA for the dredged sediment in the Keating Channel. These results verified that the model is representative of the actual conditions. It can be used as a predictive tool to estimate the total metal loads flushed from the river associated with the deposited sediments.

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Dedication

For Wazir Begum (late), Farrukh Zahid, Muhammad Zahid Mansoor, and Chaudhry Mansoor Ahmad (late).

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Chapter 1

Introduction

Population growth has caused vast expansion of the urban areas all over the world. In Canada, it is projected that in year 2100, the population will be doubled to what it was in 2000. In 2013, it was reported that 80.9% of Canada's population lived in urban areas. In Canada, urban population average annual growth rate is at 1.1% over the last five years (United Nations Statistics Division, 2015). Such rapid increase in population and its people's preference for urban settlement demands expansion of urban land. Urbanization causes a shift in the natural water cycle, reducing natural infiltration and increasing overland runoff. This impacts the receiving water bodies, which cannot withstand such drastic changes to the natural cycle. As a result, the receiving drainage channel undergoes degradation in the form of erosion due to frequent flooding, channel widening, and poor water quality due to high water temperatures and pollutant loadings from the overland runoff.

The ecological status of a river is directly related to its surrounding watershed. If the watershed draining the river is a source of heavy contamination such as heavy metals and nutrients, then its effects will be reflected in the water quality of the river (Ji, 2008). Rapid urbanization and economic growth have caused the water quality pollution and ecological deterioration to become serious problems in urban and peri-urban rivers (H. Jia et al., 2011). An increasing trend is observed in the imbalance between human needs for urbanization and sustainable ecosystem services. As the urbanization increases, runoff from these urbanized catchments increases in its metals loadings, which degrade the receiving water quality. The sources of these metals contamination in an urbanized watershed include vehicle traffic along with industrial effluents. The anthropogenic metals are zinc, copper, lead, and cadmium. These metals are dominant in urban runoff compared to untreated wastewater of a city (Yu et al., 2014).

The Don River has been labeled the 'most urban river in Canada' by Canadian Geographic (2011). It is certainly one of the largest urban watersheds in Canada, perhaps the largest. The watershed is nearly completely developed and the Don River runs right through the largest metropolitan region in the country. Not surprisingly, there is a lot of interest in understanding how sediment and pollutants such as metals move through the system. Stream restoration projects and stormwater management retrofits, and the mouth of the river are just a few of the hot spots where incomplete knowledge restricts our ability to make informed management decisions. For example, the 'Don Mouth Naturalization and Port Lands Flood Protection Project' (DMNP) has been planned, which includes establishing a floodplain within the lower reaches of the Don River. This project will, over a period of time, improve the ecological functions and provide linkages to the upstream habitats. It will also accommodate changes in precipitation and water flow and address the issues related to sediment and debris deposition and ice jams (TRCA, 2015a).

This research thesis is an effort to understand the sediments and associated metals dynamics through a river system using numerical models. The research highlights the gaps in modeling the hydrologic systems, which includes hydraulic routing, but lacks the capabilities of simulating the instream processes. Data for precipitation and flow is relatively easily monitored and commonly used for setting up these hydrologic models. However, monitoring instream sediment transport and the associated storage of pollutants in the system is extremely difficult and rarely performed.

These challenges are further motivated by the work of (Louie, 2014), who measured and compiled available information on the sediments and metals distribution trends in the Don River system. The study focused on three metals, copper (Cu), lead (Pb), and zinc (Zn) and attempted to document their spatial and temporal trends throughout the Don River system and their storage in deposited sediments. The results showed a high spatial variability of metals deposition, with river mouth showing high levels relative to the headwater location. Results of the study also highlighted the spatial and temporal limitations in obtaining detailed data on instream processes on a watershed scale, and substantiated the difficulty in understanding the movement of metal compounds and their depositional trends through the system.

A final motivation is the poor link between urban hydrologic models and hydraulic tools to model instream processes in detail, which makes the advanced hydraulic tools inaccessible for most users. Hydrologic models provide the hydraulic models with necessary loadings data for detailed instream modeling. The poor link between the two models makes it difficult to apply these hydraulic tools to assess the impact of restoration and stormwater management projects on a watershed scale. Hence, a need for a linking tool is recognized and developed as part of this research.

The trace metals studied in this research are Cu, Pb, and Zn since they are primarily sourced from the urban centers (Louie, 2014). With increasing pressure on the water resources due to expansion of urban areas, it is important to monitor the instream processes relevant to sediments and metals transport to understand the impact of restoration and stormwater management projects on these resources. This research can further enable informed decision making and infrastructure planning to mitigate the adverse impacts of urbanization.

1.1 Background

The Don River watershed is located in the Regional Municipality of York (Figure 1). The Don River flows from its headwaters on the Oak Ridges Moraine and its two major tributaries, the East Don and the West Don, flow south through the City of Vaughan and Towns of Markham and Richmond Hill. The East Don and the West Don Rivers join together on the Iroquois Sand Plain located south of the Eglinton Avenue (TRCA, 2009). The total area of the watershed is approximately 36,000 hectares. The river flows for approximately 38 Km from its headwaters on the Oak Ridges Moraine to the Keating Channel, where it drains into Lake Ontario (TRCA, 2015b).

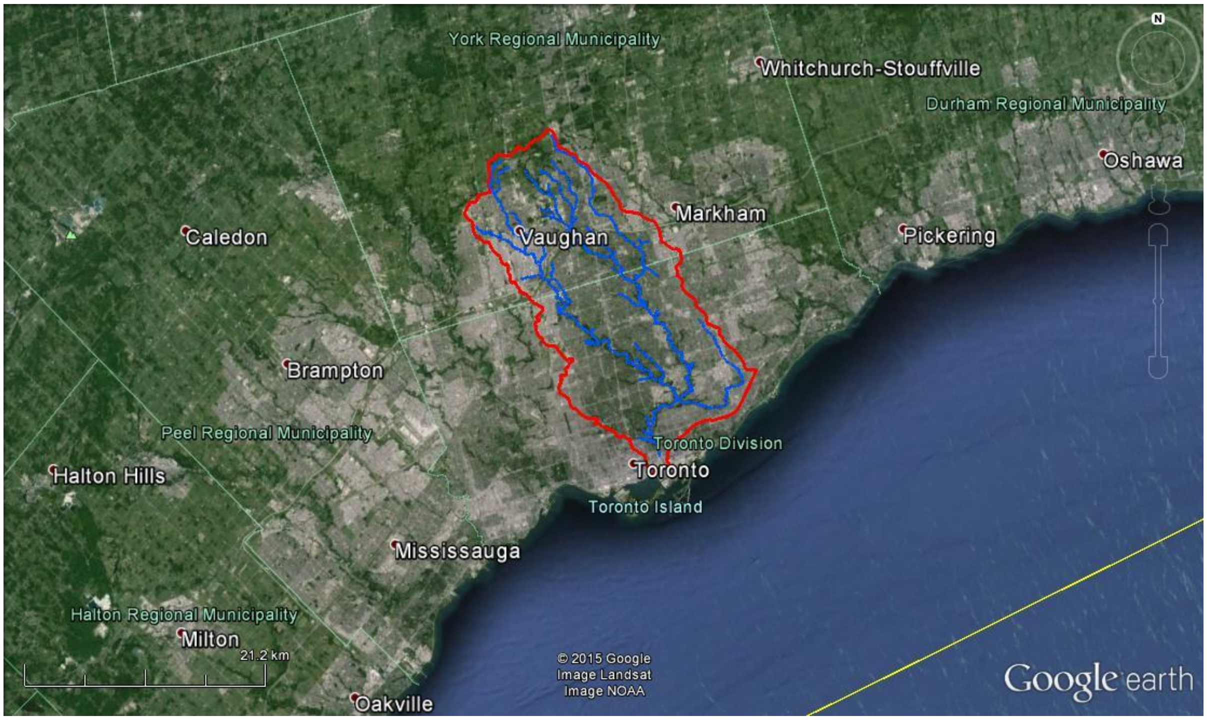

Figure 1: Location of the Don River watershed. Watershed data courtesy of TRCA and mapped using Google Earth, 2015

Mean total discharge of the Don River is 3.9m^3/s (124million m^3/year) at Todmorden (Figure 2). Baseflow accounts for 49% of the total flow of the river (TRCA, 2009). Most of the baseflow occurs from the lower catchments of the Don River watershed (TRCA, 2009) and the lower Don River is subject to high pollutant concentrations (Louie, 2014). Hence, the lower section of the Don River is the focus of this study. The study reach shown in Figure 2 extends from Taylor Creek South to the

Keating Channel and has a length of 9.81 Km obtained from scaled mapping. The study reach has confluences with two major tributaries, the East Don and the West Don.

Toronto and Region Conservation authority has monitored water quality data in the Don River since 2002 under the Regional Water Quality Monitoring Program (RWMP). It is the most recent and consistent data set available for the region, however, misrepresentation of concentration may occur due to its limited sampling frequency and coverage (Louie, 2014). The water column concentrations for total suspended solids (TSS), copper, lead, and zinc were obtained for the Todmorden monitoring station. The Todmorden monitoring station (Figure 2) is part of the RWMP network, and therefore, was used as a calibration point for the purpose of modeling the study reach.

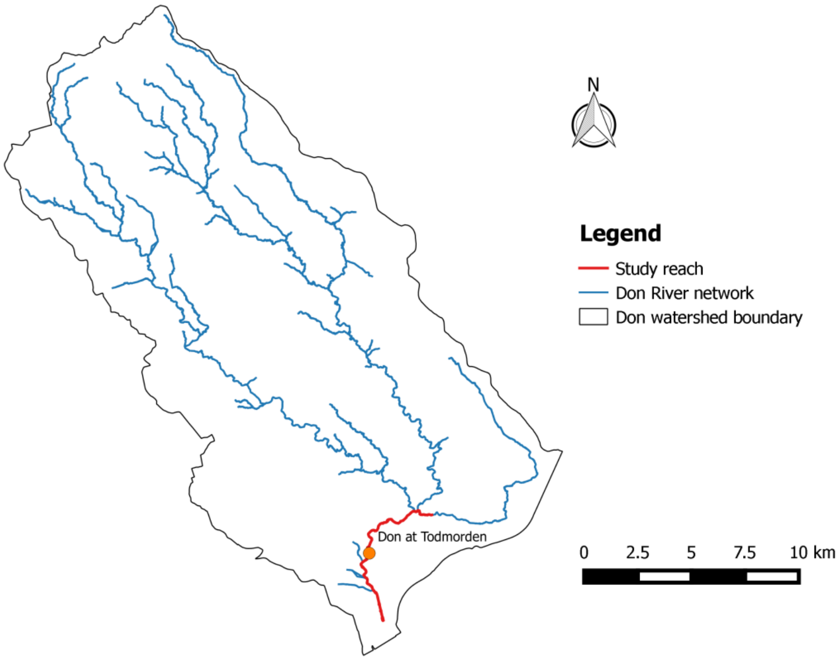

Figure 2: Location of the study reach in the Don River watershed. Data courtesy of TRCA and mapped using QGIS 2.6

Don River sediment quality is generally not monitored at the RWMP stations. However, sediment quality data may be obtained for the dredged sediments from the Keating Channel. TRCA maintains a record of pollutant concentrations in the dredged sediments from the Keating Channel along with their particle size distributions. The sediment bed concentrations for copper, lead, and zinc were obtained from the dredged sediment data. These sediment bed concentrations may be used to provide estimates of sediment pollutant loads into the Keating Channel.

1.2 Purpose and Objectives

This research aims at understanding the sediment transport and associated trace metals distribution in the lower Don River using numerical models. Both spatial and temporal distribution of total suspended sediment and the associated metals, namely copper, lead, and zinc, was simulated for the time period of May to August 2010. A 1-dimensional (1D) model was implemented for this purpose and two modeling packages were used to achieve this task – a hydrologic model called the Stormwater Management Model (PCSWMM) (James et al., 2010) and a detailed hydrodynamic, sediment transport, and pollutant fate and transport model called Environmental Fluid Dynamics Code (EFDC) (Hamrick, 1992).

The PCSWMM model was used previously by TRCA to develop a calibrated hydrologic model of the entire Don River watershed. This model did not simulate the sediment and pollutant loads from subcatchments and spanned a time period of 40 days. Hence, this model was upgraded for this study to provide non-point source loads as boundary condition data to the EFDC model. EFDC model is capable of simulating in-stream physical processes governing sediment and pollutant fate and transport in detail. Particulars regarding these modeling packages and their capabilities can be found in section 2.3.1. A need for a tool was established that can help in efficient EFDC model setup using results from PCSWMM model.

The objectives of this research are as follows:

1. Develop a tool to efficiently link PCSWMM hydrologic model results to 1D EFDC model that can be applied to any river system.
2. Use the tool to setup the 1D EFDC model and analyze the highly urban lower Don River for sediment dynamics and associated trace metals distribution, namely copper, lead, and zinc.

Chapter 2

Literature Review

2.1 Scope of Review

River dynamics and water quality modeling require understanding of the instream physical processes that govern the transport and storage of sediments and metals within a system. The simulation of metals transport and accumulation in a river is associated with sediment and water routing to and through the channel. As a result, it depends on a large number of instream processes that must be integrated in a modeling strategy. Examples of these processes include flow and sediment transport with turbulent flows in alluvial channels, mobile bed roughness, sediment settling and deposition, incipient motion, and erosion (Wu, 2008). Water quality studies, especially related to metals and solute transport, incorporate physical and chemical processes including advection and dispersion, sorption to bed and suspended sediments, transient storage, decay, and biochemical reactions (Y. Zhang & Aral, 2004). River dynamics and metals transport modeling require a theoretical understanding of these processes and their integration to represent a large system. This review provides a theoretical background of these processes and their applications in various surface water models.

Development and application of a computational model is a lengthy process which includes data preparation, parameter estimation, model calibration, interpretation of results, and uncertainty analysis. The accuracy of the model, and consequently its reliability depends on proper execution of all of these steps (James, 2002; Wu, 2008). This review compares various modeling packages available in terms of their capabilities and addresses the most suitable modeling package for the objectives of this thesis. Finally, it provides details of sediments and pollutant transport modeling applications from literature in order of relevance to the different stages of model development, thereby establishing a strategy to perform integrated hydrodynamic, sediment transport, and metals transport modeling in a coupled approach to achieve the objectives of this thesis.

2.2 River Processes

2.2.1 Hydrodynamics

Hydrodynamic processes in rivers are mainly governed by the three conservation laws – the conservation of mass, the conservation of momentum, and the conservation of energy. The mathematical equations of these conservation laws provide the basis to model hydrodynamic processes. These equations can be further modified and simplified based on the natural conditions or requirements of accuracy and efficiency. For example, the Navier-Stokes (NS) equations are derived from these laws but are impractical to apply to open channel flows because of fluid turbulence. The numerical solution of NS equation is extremely difficult due to significantly different mixing-length scales that are involved in turbulent flow. Stable solution to NS equations requires a very fine mesh resolution making the computational time infeasible for most cases. Therefore, some of the classic simplifications such as the Reynolds-averaged Navier-Stokes (RANS) equation including the turbulence models are used in computational fluid dynamics to model turbulent flows. These simplifications retain the 3D capabilities while others integrate vertically to provide shallow water 2D equations such as 2D Saint-Venant equation. Depending on the spatial dimensions of the model domain, these equations can be simplified across the entire cross-sections to get 1D hydraulic routing equation such as the Muskingum Cunge equation and the 1D Saint-Venant equation. These 1D equations are commonly used in models such as HEC-RAS (USACE, 2010), MIKE 11 (DHI, 2015), and SWMM 5 (James et al., 2010) for flood routing and calculating water surface profiles.

Some of the most common simplifying assumptions which are used in modeling open channel flows include hydrostatic pressure distribution, Boussinesq approximation, and quasi-3D approximation (Ji, 2008; Julien, 2002). Hydrostatic approximation assumes that the pressure gradient in the vertical dimension is constant and balanced by force due to buoyancy. This approximation is led by the shallow water approximation which is applicable in cases where water depth is much smaller relative to horizontal dimensions. Shallow water approximation is widely used to characterize surface waters. Boussinesq assumption states that water density is independent of water pressure which leads to the assumption of incompressible fluid. This approximation is applicable in most surface water bodies with small variations in density. Quasi-3D approximation is applied to 3D modeling applications where the concept is to treat the 3D domain in sets of horizontal layers that interact with each other via input and output fluxes. This approach eliminates the need of using momentum equation in the vertical dimension and ensures computational efficiency and accuracy (Ji, 2008). This approximation is used in the Environmental Fluids Dynamic Code (EFDC) (Hamrick, 1992). The details of this model are presented in section 2.3.1.

The combination of conservation laws including the simplifying assumptions provides a system of complex differential equations for hydrodynamic modeling. The level of detail required can drastically change the computational time needed to numerically solve these equations. Hence, mesh resolution becomes a significant factor to numerically solve these equations over large domains and time periods. Various numerical discretization schemes are used which include finite element, finite difference, and finite volume methods to solve the system of governing differential equations. The derivations of the equations of fluid flow for hydrodynamic modeling are presented in (Julien, 2002) and (Ji, 2008) and their numerical discretization and schemes are explained in (Wu, 2008).

2.2.2 Sediment transport

There are four basic processes associated with transport of sediments. These are resuspension and erosion of the sediment bed, transport of sediment in the forms of bed load and suspended load, settling and deposition, and consolidation of the sediment bed (Ji, 2008). The resuspension and erosion, commonly called ‘entrainment’ or the ‘initiation of motion’, is usually modelled as a function of either shear stress or drag exerted by the flow on the bed. Entrainment occurs when the applied shear stress due to the flow exceeds a critical threshold value. The concept of critical Shield’s stress is widely used to model incipient motion of particles. It is a dimensionless parameter, a function of particle diameter and density, and is used in various sediment transport equations as a threshold value for incipient motion. Transport of sediments occurs in the form of bed load and suspended load when the applied shear stress levels are within the range required for transport. Settling and deposition takes place when the sediment transport capacity of the flow is exceeded, or the applied shear stress becomes lower than the critical shear stress for deposition. Consolidation of the sediment bed is a relatively long term process and occurs usually in deep water bodies such as lakes, providing sufficient weight for the bed to consolidate. Therefore, sediment transport is a function of hydrodynamics processes along with sediment properties such as particle size, density, shape and composition.

Sediment transport occurs in two phases, the bed load and the suspended load. Bed load transport includes rolling, sliding, saltating or jumping, and in suspension near the bed surface. It takes place in a thin layer above the bed surface and moves in continuous contact with the bed. The motion is mainly governed by shear stress exerted by the flow. Bed load is significant in non-cohesive sediment transport in terms of bed forms such as ripples, dunes, and bars which may affect the flow conditions and also contribute to channel migration. It is also important for sorting and reordering of the particles and size-class fraction within a channel. Multiple bed load sediment transport formulas have been developed. The ones which are most widely used are Meyer-Peter and Muller (1948), Bagnold

(1956), and Van Rijn (1948). These formulas are a function of excess shear stress which causes the bed sediment in motion and are explained in (Julien, 2002) and (Ji, 2008). It is to be noted that none of these formulas are recognized as adequate for determining bed load transport and as a result, the formula providing the closest results to actual transport rates is considered representative. The suspended load involves particles within the water column above the thin layer of bed load transport. These suspended sediments are commonly referred and reported as total suspended solids (TSS) per unit volume of water. The suspended solids are commonly modelled using the mass conservation used for solute transport. Cohesive and non-cohesive particles in the water column are transported through the same principle of advection, dispersion, and settling (Ji, 2008).

Settling is controlled by the particle diameter, density, and viscosity of the fluid, which are used to calculate the settling velocity of a given grain size to model this process. It is used in suspended sediment transport formulation and the settling particles contribute to the deposition process, which further leads to consolidation of the bed based on flow and bed conditions. Sediment bed models are based on the mass conservation of sediment in a bed control volume. The sediment bed is discretized into layers and the mass conservation laws are applied in 1D in the vertical. The sediment bed model is usually coupled with the sediment transport model to update the deposition and erosion fluxes based on flow and bed conditions. Calculation of bed elevation change follows from this coupling and is obtained by solving the sediment continuity equation, also called the Exner equation, for bed surface layer (Bai & Duan, 2014; Ji, 2008). Therefore, settling, deposition, and resuspension are the key instream processes, which are coupled with the hydrodynamic processes governing the sediment transport simulation.

2.2.3 Water quality

The key processes that govern the fate and transport of pollutants include sorption and desorption to particulates in water column and the sediment bed, settling and resuspension of particulates, diffusion between water column and sediment bed interface, and the removal processes. Mass conservation equation is used to model contaminant transport incorporating these physical processes (Ji, 2008; Trento & Alvarez, 2011). A complete schematic for these processes is shown in Figure 3, which highlights the general environmental pathways of a pollutant in a surface water body.

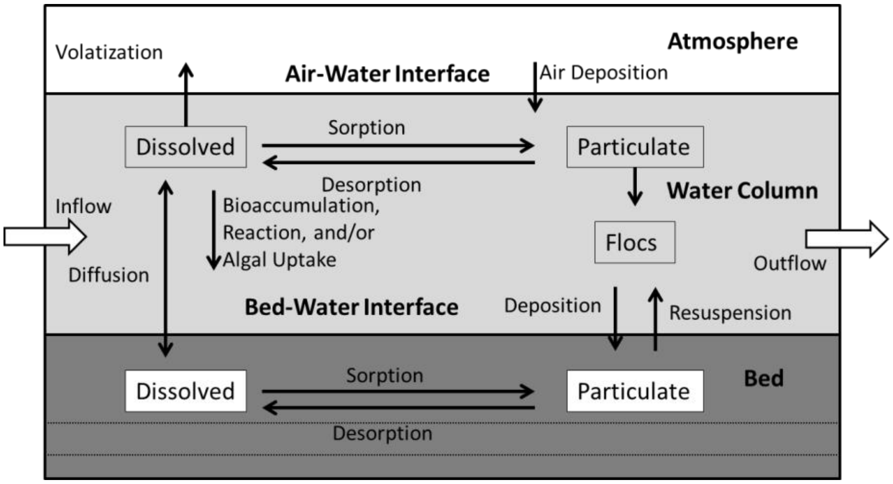

Figure 3: Fate and transport processes of a toxicant. Adapted from (Ji, 2008)

Metals in a water body can undergo series of complex processes including advection and dispersion and can be transported by inflows, outflows, and deposition and resuspension of sediments, which are all associated with hydrodynamic transport processes (Chu & Rediske, 2012). Interchange between particulate and dissolved states in both the water column and the sediment bed occurs through sorption and desorption processes. Dissolved contaminant in the pore water of the bed can diffuse to and from the water column depending on the concentration gradient between the two compartments. Furthermore, burial into the deep sediment layer, volatilization, chemical transformation, and bioaccumulation are all removal processes of contaminants from the system. The selection of processes for contaminant fate and transport modeling is based on the properties of the contaminant being studied, the spatial and temporal scale of the model, and the required complexity (Ji, 2008).

Sorption (or adsorption) and desorption is a major process influencing the concentrations of metals. Sorption to solid sediment particles is an influential pathway for the transport of metals and other contaminants in natural water bodies. Hence, the metal concentration is affected by the transport, deposition, and resuspension of sediments. On the other hand, desorption is the process by which these metals are entrained into the aqueous phase from the particulate phase. Sorption and desorption are known to be relatively fast compared to other processes such as decay and reactions, and are assumed to undergo instantaneous equilibrium. Partitioning coefficients are used to model the sorption processes and are given as the ratio of sorbed metal concentration (mg metal per Kg sorbing material) to dissolved metal concentration at equilibrium (mg per liter of solution) (Allison & Allison, 2005; Ji et al., 2002; Wang et al., 2013). Sorption isotherms are derived from these partition coefficients, which are empirical models obtained from experimental data. The most common sorption isotherms are linear isotherm (Henry's adsorption isotherm), Freundlich isotherm (1909), and Langmuir isotherm (1916). The aqueous or dissolved contaminants are directly related to environmental degradation and poor water quality, whereas, particulate phase does not pose a significant threat to the environment and are considered biologically inactive. It is important to note that sorption of contaminants is mostly linked to smaller size particles such as silt and clays due to their high surface area to volume ratio as compared to large particles such as sand. Moreover, smaller particles are relatively more mobile under variable flow conditions. Hence, the behavior of contaminants is closely linked to the transport of small sediment size classes (Ji, 2008).

A reliable and representative contaminant transport model requires an appropriate hydrodynamic and sediment transport model that can be integrated to simulate the instream contaminant transport processes (Ji et al., 2002; H. Jia et al., 2011). In fact, hydrodynamic and sediment transport models are pre-requisites to perform contaminant transport modeling that covers the key instream processes of deposition and resuspension along with sorption and desorption of contaminants. A modeling package containing a contaminant module that is well-coupled with the hydrodynamic and sediment transport modules will provide adequate representation of the instream conditions of a given channel.

2.3 Models of River Dynamics

2.3.1 Description of existing models

Various integrated river models were reviewed for the purpose of selecting the most suitable modeling package to achieve the hydrodynamic, sediment transport, and metals dynamics simulation in a coupled approach. Table 1 lists and compares these modeling packages using relevant description of the underlying processes and linkages to other models. Some of the models, such as HEC RAS, are widely used in 1D river engineering applications, while others such as EFDC Explorer and MIKE11 are used for detailed research on sediments and water quality constituents in a river system. The criteria for the selection of a model for this research are based on the underlying physical processes and its integration and linkage capacity with other modules. Moreover, the level of detail required in terms of spatial resolution and dimensions also played a decisive role in selecting a suitable model. Models such as CCHE2D and Morpho2D are dedicated to depth-averaged reach scale analysis of a system, while other such as HEC-RAS can be applied to 1D channel networks. The integrated hydraulic models are based on the conservation laws and instream physical processes incorporating various simplifying assumptions, based on the dimensionality and scope of the model. Table 1 provides a basis to select the most suitable hydraulic model that can be used to simulate hydrodynamics, sediment transport, and associated metals dynamics in an integrated manner, and which can be linked to a suitable hydrologic model to provide necessary loadings of sediments and metals from non-point sources (NPS).

The Hydrologic Engineering Center (HEC) of the US Army Corps of Engineers (USACE) developed a hydraulic model called HEC-RAS for 1D simulation of natural and constructed channel networks. HEC-RAS is capable of performing steady and unsteady flow simulations using 1D energy loss equation for steady flows and fully dynamic 1D Saint-Venant equation for unsteady flow regimes to calculate water surface profiles. It also performs sediment transport (movable boundary) computations, water quality analysis, and several hydraulic design computations in an integrated manner under the same geometric domain. The water quality module of HEC-RAS simulates a limited set of water quality constituents through the 1D advection-dispersion equation using a control volume approach. The water quality constituents that can be currently modelled in HEC-RAS include dissolved nitrogen (NO_3-N, NO_2-N, NH_4-N, and Org-N), dissolved phosphorous (PO_4-P, Org-P), algae, dissolved oxygen (DO), and carbonaceous biological oxygen demand (CBOD) (USACE, 2010). It does not support an exclusive metals fate and transport module and does not have a GIS interface to link a hydrologic model.

A hydrologic model called the Hydrologic Simulation Program-Fortran (HSPF) (Bicknell et al., 1997) simulates the hydrologic and associated water quality processes on pervious and impervious land surfaces and well mixed impoundments for extended time periods. It is primarily intended for rural and agricultural watersheds and uses continuous meteorological data to compute streamflow hydrographs and pollutographs. The model simulates a variety of hydrologic processes ranging from infiltration, snow melt, baseflow, interflow, and groundwater interactions along with water quality processes for dedicated ecological studies. It uses a wide range of parameters and is generally applied to assess the impacts of land-use change on point and non-point source (NPS) loads of water quality constituents for ecological studies. The NPS loads for various water quality constituents can be used to perform detailed instream modeling of a channel using dedicated hydrodynamic and water quality models such as EFDC (Hamrick, 1992) and WASP (Ecosystems Research, 2013b).

Environmental Fluids Dynamics Code (EFDC) developed by (Hamrick, 1992) is a general-purpose model which has been applied for simulation of 1D, 2D, and 3D flow, transport, and biogeochemical processes in surface water systems. Dynamic Solutions-International, LLC (DSI) has developed a user interface for EFDC called EFDC Explorer for pre and post processing of the model (Craig, 2015). The model has a wide range of application to rivers, lakes, estuaries, reservoirs, wetlands, and coastal regions for hydrodynamics, sediments, metals, and water quality analysis and is currently used by academic institutions for research purposes and other organizations and consultants (Guo & Jia, 2012; Ji et al., 2002; H. Jia et al., 2011). The model can be easily applied to 1D or 2D studies by using 1D or 2D model grid without any changes to the source code. The grid can either be in cartesian coordinates or can be orthogonal curvilinear to represent complex geometries. It does not have a built-in GIS linkage to a hydrologic model for grid generation and boundary loadings allocation. EFDC was originally developed at the Virginia Institute of Marine Science and is supported by United States Environmental Protection Agency (U.S. EPA). The model has four major sub models which are a hydrodynamic model, a sediment transport model, a toxic model, and a water quality model. All these sub models are fully integrated which makes it a unique suite for modeling of surface waters. There is no need of developing a coupled interface between various sub models to represent different processes. A recent update of the model includes a module to simulate submerged aquatic vegetation which links with the hydrodynamic, sediment transport, and water quality modules (Ji, 2008). EFDC Explorer also includes an interface for performing water quality simulation using WASP model (Ecosystems Research, 2013b), linking the hydrodynamic and sediment transport results. It also provides an interface to link HSPF hydrologic model (Bicknell et al., 1997) for providing loadings data to the hydrodynamic, sediment transport, and water quality model.

The hydrodynamics module of the EFDC solves the vertically hydrostatic, free-surface, turbulent-averaged equations of motion for a variable density fluid. Transport equations for turbulent kinetic energy, turbulent length scale, salinity, and temperature are also solved. Multiple size classes of cohesive and non-cohesive suspended sediment including bed deposition and resuspension is simulated by the sediment transport module. It also simulates bed geo-mechanics and the deposited bed can be represented by multiple layers. The elevation changes between water column and sediment bed interface are incorporated into the hydrodynamics equations. Furthermore, EFDC toxic module simulates the fate and transport of multiple toxic chemicals such as metals with full integration with the hydrodynamics and sediment transport modules. Metal concentrations are calculated in the water column and the bed using the equilibrium partitioning coefficients between dissolved and particulate phases. The processes include deposition and associated surface water entrainment, resuspension and associated pore water entrainment, pore water expulsion due to consolidation, and diffusion between surface water and pore water phases. A built-in water quality and eutrophication module simulates 22 state variables in the water column and is coupled with a 27-state variable sediment diagenesis model (Ji, 2008).

PCSWMM is a GIS based user interface that runs the EPA SWMM5 hydrologic model. It is especially designed for urban watersheds and has the capability to perform overland runoff simulation from precipitation data along with buildup and wash-off simulations for pollutants. Its built-in GIS tool can be used to assign land use data for various subcatchments to perform pollutant buildup and wash-off calculations. EPA SWMM5 model has the option of kinematic and dynamic wave routing using Saint-Venant equation for hydraulic simulations through the river network. However, it cannot simulate in-stream sediment and contaminant transport processes which involve erosion, deposition, diffusion, and contaminant sorption to sediments etc. It simply routes the water quality constituents using complete mixing or plug flow assumption (James et al., 2010). Modeling of such physical processes require a specialized integrated model that couples hydrodynamic, sediment transport and contaminant fate and transport simulation such as the EFDC model.

Deltares Systems have developed integrated modeling packages for simulation of hydrodynamics, sediment transport and water quality processes. One of the software packages, SOBEK, is a powerful modeling suite for flood forecasting, optimization of drainage systems, sewer overflow design, river morphology, salt intrusion, and surface water quality. The model can be applied to complex systems in 1D network grids with internal loops and branches and on 2D horizontal grids. The hydrodynamics code uses complete Saint-Venant equations with capabilities to simulate steep channels with super critical flows and moving hydraulic jumps. Sediment transport capacity simulations are available within the hydrodynamic module, however, no dedicated morphological module is integrated. The water quality module can simulate any water quality variable with its associated processes. The module is equipped with a library of 900 processes and substances, including eutrophication, sorption, heavy metals, and micro-pollutants which can be applied to specialized problems (Deltares System, 2012).

Deltares Systems also developed a suite for 2D and 3D simulation of fully integrated processes including flow, sediment transport, and water quality. This suite is called Delft3D and is particularly meant for detailed studies of surface water bodies such as lakes and estuaries. The hydrodynamic module solves unsteady flows incorporating variable fluid densities, tides, winds, air pressure, waves, and turbulence. The suite uses curvilinear and rectilinear grids under the assumption of hydrostatic flow. Sediment transport module computes both suspended sediment and bed load transport for cohesive and non-cohesive fractions. The morphology module is fully integrated with the hydrodynamics module and suspended sediment is computed using advection-diffusion solver of the flow module. The water quality module incorporates the same library of processes and state variables as the SOBEK suite described above (Deltares Systems, 2012).

A complete 1D river modeling suite called MIKE 11 developed by Danish Hydraulic Institute (DHI) includes hydrodynamic, sediment transport, and water quality module for integrated river modeling. MIKE 11 does not have a GIS interface, but it links with a built-in urban hydrologic module for coupled runoff and hydrodynamic simulation. However, sediment and pollutant loads from catchments in urban runoff are not supported. MIKE 11 uses solutions to fully dynamic Saint-Venant equations for unsteady flow routing, while Muskingum Cunge routing option is also available for simplified channel routing. MIKE 11 has a specialized sediment transport module representing erosion, deposition and morphological changes of river bed bathymetry. It also includes an advection-dispersion solver for transport modeling of conservative pollutants with a linear decay option. It also has an integrated water quality module dedicated for ecological studies applying water quality processes and reactions throughout the river system (DHI, 2015).

Another complete modeling suite by the name of CCHE2D was developed at the National Center for Computational Hydroscience and Engineering (NCCHE), University of Mississippi. CCHE2D is a depth-integrated two-dimensional hydrodynamic and sediment transport model for unsteady open channel flows in alluvial systems. The hydrodynamic model is based on depth-averaged Navier-Stokes equation with Boussinesq's approximation for turbulent shear stresses. The sediment transport model calculates non-equilibrium transport using advection-diffusion equation of the suspended load and continuity equation for bed load transport. The bed sediment sorting is also enabled in the model where bed material is divided into several layers. The model can simulate flow and sediment transport either simultaneously or independently depending on the bed change response to flow dynamics. A pollutant transport module has been recently developed called CCHE2D-CHEM which assumes linear equilibrium sorption and first-order decay reactions. A water quality module called CCHE2D-WQ is also developed for instream ecological and eutrophication modeling. Vertical diffusion and mass exchange between water column and bed is also considered (Y. Jia, 2012). The model is particularly dedicated for depth-averaged 2D applications and has not been tested on a large river network with branches and loops (Y. Zhang, 2005). CCHE 1D is a 1D hydrodynamic and sediment transport model developed by NCCHE for simulation of large river networks. It does not have an integrated 1D contaminant transport module which is the subject of future development. CCHE 1D uses a watershed-based approach providing integration with overland runoff. However, it has a GIS-based graphical interface requiring a separate GIS package for its setup, which is now outdated. A new interface for GIS linkage is under development for CCHE 1D modeling suite.

A software package called International River Interface Cooperative (IRIC) was developed by Professor Yasuyuki Shimizu of the Hokkaido University and Dr. Jon Nelson of United States Geological Survey (USGS). IRIC is a river flow and river bed variation analysis software package providing an interface for multiple solvers to analyze river flow and river bed dynamics. The solvers include FaSTMECH, Nays2D, River2D, ELIMO, Morpho2D, etc. These solvers use the same conservation laws of mass and momentum with various simplifying assumptions described in section 2.2. For example, the FaSTMECH (Flow and Sediment Transport with Morphological Evolution of Channels) solver uses the conservation of mass and momentum with hydrostatic assumption, Reynold’s stresses and turbulence closure schemes. It employs cylindrical coordinate system and a quasi-steady approximation, allowing the simulations over long timeframes (Nelson, 2010). These solvers are capable of solving flow and sediment transport problems and most of them are dedicated to 2D applications (IRIC Project, 2010). Although IRIC provides a useful tool to analyze river flow and channel morphology, it does not provide dedicated water quality and contaminant transport capabilities. Therefore, the application of such solvers may require coupling of an independent water quality model such as Water Quality Assessment Simulation Program (WASP) (Ecosystems Research, 2013b) to perform integrated flow, sediment transport, and water quality simulations.

WASP is a dynamic compartment-modeling program for surface water systems to investigate water quality related to ecological studies. It simulates water quality transport processes in both the water column and the underlying benthos. WASP is flexible in its application to 1D, 2D, and 3D systems, and to simulate a variety of pollutant types. The state variables involve conventional pollutants such as nitrogen, phosphorous, dissolved oxygen, BOD, sediment oxygen demand, and algae along with organic chemicals, metals, and pathogens. The fate and transport processes that are represented in the model include advection-dispersion, point and diffuse mass loading and boundary exchange. WASP can be linked with hydrodynamic and sediment transport models that can provide flows, depths velocities, temperature, salinity and sediment fluxes for integrated surface water modeling (Ecosystems Research, 2013b).

Another model by the name of One-Dimensional Riverine Hydrodynamic and Water Quality model (EPD-Riv1) is applicable to 1D channel networks for hydrodynamic and water quality simulations related to nutrients cycle through its linkage with WASP model. It is suitable to 1D river systems that do not involve sediment transport, toxics, or metals (Ecosystems Research, 2013a).

Table 1: Summary of models for river dynamics simulation

Models	**Hydrodynamics**			**Sediment transport**	**Water quality**
	1D	**2D**	**3D**		
Hydraulic models					
HEC RAS	✓			dedicated sediment transport module, no GIS linkage and interface to hydrologic model	advection-dispersion module, no support for metals transport
EFDC Explorer	✓	✓	✓	dedicated sediment transport module, interface for HSPF data import, no GIS linkage	fully integrated dedicated module for metals transport, links to WASP
SOBEK	✓	✓		no dedicated sediment transport module	dedicated water quality module, includes metals
Delft3D		✓	✓	morphology module, fully integrated	dedicated water quality module, includes metals
MIKE 11	✓			dedicated sediment transport module, no sediment loads estimation through coupled hydrologic module, no GIS linkage	coupled advection-dispersion module for conservative pollutants, dedicated ecological module
CCHE 1D	✓			dedicated sediment transport, applies to dendritic networks	no dedicated toxic transport module for 1D application
CCHE 2D-CHEM		✓		dedicated sediment transport, reach scale	dedicated toxic transport module
CCHE 2D-WQ		✓		dedicated sediment transport, reach scale	dedicated water quality module
Nays		✓		riverbed variation, lateral erosion, reach scale	no pollutant transport
FaSTMECH		✓		riverbed variation, reach scale	no pollutant transport

Models	Hydrodynamics			Sediment transport	Water quality
	1D	**2D**	**3D**		
River 2D		✓		no sediment transport, reach scale	no pollutant transport, customized for fish habitat studies
Morpho 2D		✓		riverbed variation, reach scale	no pollutant transport
EPD-Riv1	✓			no sediment transport, applies to dendritic networks	no metals and toxic simulation, links to WASP model
WASP	✓	✓	✓	no sediment transport	dedicated water quality model, requires linkage with hydrodynamic models such as EFDC
Hydrologic models					
HSPF	✓			rural hydrologic model, provides sediment loads from NPS, no dedicated instream transport model	provides pollutant loads from NPS, no dedicated instream transport model
PCSWMM	✓	✓		urban hydrologic model, provides sediment loads using buildup/wash-off models, no dedicated instream transport model, built-in GIS interface	provides loads based on buildup/washoff models and co-fractions approach, no dedicated instream transport model, built-in GIS interface

From the comparison of different models, it can be concluded that there is a general lack of models dedicated to sediment and metals fate and transport in urban environments. It is not clearly understood how these sediments and metals are routed through the catchment and whether they are accumulating at certain locations where deposition is prevalent. This is particularly true in urban catchments, where there are even fewer models despite the need for understanding the movement of sediments and metals, and using that understanding to make rational decisions about restoration and stormwater management. PCSWMM provides an urban hydrologic model with a capability to estimate pollutant loads to the river network through buildup and wash-off models. A hydrodynamic model such as EFDC include a dedicated instream metals transport module, but does not have an interface to link an urban watershed model (PCSWMM) that can provide the NPS metal loadings to the channel domain. It provides an interface to import HSPF results, but HSPF is not dedicated for urban watershed modeling, making it unsuitable for metals analysis. EFDC Explorer is considered most suitable commercially available modeling package for the purpose of simulating instream metals transport for this research. It has flexibility to be applied to a 1D domain with coupled sediment and metals simulation. However, a need of an efficient and specialized linkage tool is identified which can automate the process of linking the urban hydrologic model (PCSWMM) to EFDC model.

2.3.2 Applications

This section is intended to provide examples and case studies of integrated modeling applications as described in literature. These case studies represent a wide range of hydrodynamic, sediment, and contaminant modeling applications, and therefore, are addressed to provide a general perspective of handling different stages of model development. The following subsections have been organized in an order of model setup in terms of boundary conditions, initial conditions, spatial and temporal discretization, and model calibration and validation. Each stage of model development is supported with case studies from cited literature providing description of model application for the integrated study of hydrodynamics, sediment, and contaminant transport.

2.3.2.1 Boundary conditions

Reliability of the model depends on accurate set up of boundary conditions required to run the model. Boundary conditions are usually inflow and outflow information with flows at upstream boundaries of all tributaries, lateral inflows from groundwater or runoff and flow diversions. It is recommended to use a hydrologic model to determine inflows and non-point source loadings during storm events (Ji, 2008). Numerical simulation of open channel networks, water quality, and sediment dynamics requires accurate estimation of runoff and sediment transport rate from the catchment. These are two important factors to the design of hydraulic structures or river restoration. There are several rainfall-runoff models which exist, such as PCSWMM designed specifically for urban catchments. However, they do not use the specific sediment transport equations to simulate sediment transport from the watershed (Chen et al., 2011).

A few modeling studies (Bai & Duan, 2014; Hu et al., 2011; Ji et al., 2002; W. Zhang et al., 2014) used the most basic approach of applying the observed data in the form of hydrographs, rating curves, and concentration time series for providing the boundary conditions to the numerical models. For example, a modeling exercise by (Ji et al., 2002) adopted the EFDC model to simulate 77 Km reach of the Blackstone river which has six tributaries and a drainage area of 1657 Km^2 including 30 cities and towns. The calibrated Blackstone River model was used to investigate the contribution of point sources, non-point sources, and resuspension process to the sediment and metal concentrations. The modeling study was event based and data from 3 storm events at 16 stations with 4-hour temporal resolution was used. Five metals were simulated namely cadmium, chromium, copper, nickle, and lead. The model was developed to study sediments and heavy metals interaction and used the observed data from Blackstone River initiative (BRI). BRI data was the result of extensive study on the Blackstone River conducted by US EPA. Therefore, due to extensive short-term high resolution data available for the entire river and its six tributaries, whole sediment and metal transport could be simulated with high accuracy. Very few modeling studies have comprehensive datasets for extensive calibration and validation of the model and for providing boundary conditions. However, this study recognizes that accumulation of contaminants and sediment on the river bed is a long-term process of years and decades. Therefore such small high-resolution data sets should not be used for long-term investigation of sediment deposition and contaminant accumulation on river bed (Ji et al., 2002). This necessitates the use of a watershed model to provide adequate boundary conditions over long time periods.

An approach to apply boundary conditions in an integrated modeling application to a river with branches was given by (H. Jia et al., 2011) in an attempt to describe rehabilitation solution for Nansha River, Beijing. Nansha River is a peri-urban river located in the northern part of Beijing metropolitan area in Haidan district. Nansha River is heavily polluted with BOD5, ammonia and total phosphorous because of untreated waste water discharge into the river. Therefore, a water pollution control plan was drafted for the local authority in an attempt to rehabilitate the water environment of Nansha River. This was achieved through coupled hydrodynamic and water quality modeling with scenario analyses over a long time period.

EFDC model was used for this purpose for hydrodynamic simulation coupled with WASP/EUTRO model for water quality simulation. Nansha River has several tributaries, sluices, and rubber dams. The main stem of the river is 17 Km long. A watershed model of the region, which was previously developed in SWAT, was used to apply flow data at the tributary junctions as the input boundary condition for EFDC hydrodynamic model. Boundary conditions for the water quality model in different hydrological years were calculated based on land use information and GIS application by incorporating the export coefficient model (ECM). The export coefficient model is an empirical tool to estimate total annual loads of nitrogen and phosphorous delivered to any given sampling site from its catchment (Ding et al., 2010; Johnes, 1996). Point source flows and loads were based on wastewater treatment plant schemes. The inflow hydrographs from SWAT and pollutant loads from ECM were applied at the tributary junction at the respective grid cell. Such an approach for the set-up of boundary conditions provided reasonable results in terms of channel network modeling. The model was validated and applied successfully for various scenarios. These scenarios involved change in nutrient loadings from the catchments through varying land rehabilitation schemes (H. Jia et al., 2011).

In another study to address the challenge of providing accurate boundary conditions from large watersheds, a physical soil erosion deposition model (PSED) was developed to simulate runoff, sediment yield and erosion in watersheds (Chen et al., 2006). PSED model incorporates suspended sediment transport, bed load transport, entrained and deposited sediment in the continuity equations. The model is applied to each computational cell which represents a homogenous landscape using a geographic information system (GIS) tool. No other simplification in the hydrologic or physiologic parameters is attained which makes PSED model very reliable for simulations of runoff, suspended sediment transport, and sediment yield over large catchments with multiple watersheds. The model uses the observed precipitation data to simulate runoff and suspended sediment concentration hydrographs, along with soil erosion and deposition patterns and sediment yield. It has been successful in providing accurate boundary conditions for flow and suspended sediment concentrations, along with sediment yield for large catchments (Chen et al., 2006; Chen et al., 2011).

As inferred from various examples mentioned above, multiple approaches exist for the setup of boundary conditions in an integrated modeling application. It is to be noted that the best approach depends upon the availability of the resources and the requirements of the modeling exercise. For example, developing a watershed model to estimate non-point source loads for runoff, sediments, and heavy metals may be a recommended approach for long term analysis of sediment dynamics and associated accumulation of heavy metals pertaining to lack of such extensive data.

2.3.2.2 Initial conditions

The importance of initial conditions is described by (Bussi et al., 2014) in an attempt to analyze the effects of initial sediment conditions on model accuracy. The authors recognize the fact that the effect of initial sediment availability have not been very well documented and therefore, a need for a dedicated modeling exercise is observed to quantify the impacts of initial sediment availability.

The “warm-up” or “spin-up” simulation refers to running the model for a specified long time period using arbitrary initial conditions and using the results at the end of the simulation period as the “new” initial condition for model runs. Continuous simulation models such as groundwater models require initial conditions which are usually provided by running warm-up simulations for initial soil moisture content and groundwater levels. However, initial availability of the sediments is dependent upon previous extreme events, and therefore, warm-up simulation time periods are difficult to establish. Automatic calibration of the initial conditions requires numerous model runs which can significantly increase the computational burden and reduce efficiency. Furthermore, if a short time period on a scale of few storm events is used for calibration, the effects of initial sediment conditions on model results can be profound (Bussi et al., 2014).

(Bussi et al., 2014) used three strategies to assess the impact of initial conditions in their research. Strategy 0 implied zero initial sediment availability, strategy 1 represented manual calibration of initial conditions, and strategy 2 referred to warm-up simulation for estimating initial sediment conditions. It was concluded that considering the sediment hydrographs and total volume production, all three strategies provide satisfactory and similar results with no systematic bias (Bussi et al., 2014).

A modeling exercise by (Ji et al., 2002) adopted the EFDC model for Blackstone River to assess the EFDC model for 1D analysis of sediments and heavy metals. The modeling exercise was conducted on short time scale of a few storms as available BRI data was high resolution spanning a few storm events. The initial conditions for hydrodynamic model were set by running a 60-day simulation prior to the calibration phase. The initial bed sediment conditions were first set to be uniform along the river pertaining to lack of sediment core data. A constant active sediment layer depth was assigned. For metals simulation, a single constant initial bed sediment concentration of 10mg/Kg was specified for all the metals. A 60-day warm up simulation was conducted to reduce the impact of bed initial conditions on model results. The results were presented with statistical analysis between observed and simulated data and showed good agreement.

Similarly, a modeling exercise by (Hu et al., 2011) used a coupled 1D (Riv 1D) and 3D (ECOM) hydrodynamic and sediment transport model to study the mass flux budgets of water and suspended sediments for the Pearl River Delta in China. The study used 60-day warm-up simulations for initial hydrodynamic conditions and 30-day warm-up simulation for initial sediment conditions. The model was run for short-term simulation of 10 days each for calibration and validation based on available monitoring data. The results of the model were deemed acceptable based on statistical analysis with the observed data.

The recommended approach to set up initial conditions as used in several modeling applications explained above is running the warm-up simulation in case of no available observed data for initial conditions. This ensures that the effect of initial conditions on the model output is minimal, especially in the case of short-term simulations on a scale of a few storm events. For long-term continuous models over the period of years to decades, the effect of initial conditions on model outputs is not significant, however, warm-up simulation is still recommended.

2.3.2.3 Spatial and temporal discretization

The governing equations used to define the hydrodynamic, sediment transport, and water quality processes in water bodies are derived for a three-dimensional representation of the aquatic environment. However, geometric dimensions allow for certain simplifications in these governing equations which are required for efficient solutions to these complex equations saving the computational cost. Therefore, a numerical model should incorporate the dimension in which the spatial variability is most significant in terms of the simulated processes (Ji, 2008). Finer spatial resolution also leads to a finer temporal resolution for numerical stability. Hence, model discretization is significant in term of model efficiency and accuracy and is often determined by the requirement of the modeling exercise and the simulation time period of the model.

Blackstone River modeling for sediments and metal transport was conducted using a 1D grid in EFDC by (Ji et al., 2002). It is the first application of EFDC to a 1D system. One of the purposes of the study was to investigate the flexibility of EFDC model to 1D application. The Blackstone River is small and narrow which justifies the use of one grid cell across the river. Moreover, the river is shallow with flow velocities in the range of 0.3m/s to 1.0m/s and is well-mixed in the vertical dimension. Therefore, one layer was used in the vertical direction which was deemed acceptable. The 77 Km reach of the Blackstone River was modelled using 256 grid cells with varying cell widths along the river and a uniform length of 300m. This is also referred to as a curvilinear orthogonal grid system as it represents the geometric boundaries of the river. The time step used for the simulation of three storm events spanning 168 days was 30 seconds. Such a fine temporal resolution is adopted because of the available high-resolution data from the Blackstone River Initiative (BRI) which complements the output results of the model.

Similarly, the study conducted by (H. Jia et al., 2011) using the EFDC software to model the Nansha River in Beijing for water quality pollutants used 1D grid to represent the river system. The 17 Km reach of the Nansha River with several flow control structures was modelled using 62 cartesian horizontal grid cells. The length of the grid cells was set to be 300m which is the same used by (Ji et al., 2002; Ji, 2008) to model the Blackstone River. The width of the Nansha River ranges from 40m to 100m with average depth of 2.5m to 4m. These geometric dimensions of the river justify the use of 1D grid to represent the associated physical processes. The temporal resolution was set at 1 day for input time step of flow and pollutant loads. The same temporal resolution was used for the reporting of the model results. A remarkable difference in time frames can be noted between this study and the Blackstone River model developed by (Ji et al., 2002). This difference is due to the different objectives of the two models. The Nansha River model simulates long term scenarios over a time span of three years intended for river rehabilitation through various land use schemes. This allows for a coarser temporal resolution to represent the associated processes. Moreover, it is suggested that modelling of sediments and associated metals should be performed over long time scales, as accumulation of sediments and contaminants on the river bed is a long-term process of months or even decades (Ji et al., 2002). Therefore, for such long time periods of simulation, a coarse temporal discretization is required for efficient and cost effective analysis.

There are several applications of EFDC modeling software where complete 3D models were developed based on the requirements of the modeling results, geometric features of the concerned water body, and the available data (Huang et al., 2008; Wang et al., 2013). These 3D models are usually applied to lake, estuaries, and river deltas for accurate representation of such domains. The simulation time periods vary from a few storms to months depending on the availability of resources and study requirements.

Importance of 1D hydrodynamic, sediment transport, and contaminant modeling was emphasized in a study by (Trento & Alvarez, 2011). The study suggested the 1D grid is adequate for rivers with length-to-width ratio of 10 or higher. Moreover, it emphasized that a 1D model can be an efficient cost-saving tool in engineering analyses and decision making.

From the review of the past application of the coupled models, it can be deduced that 1D models are applicable to shallow river reaches with a length-to-width ratio of 10 or higher. Moreover, the selection of spatial and temporal discretization is a function of geometric configuration of the water body, available resources in terms of time and observed data, and the requirements of the model results. Model dimensionality and discretization (or model complexity) should be set in accordance with the feasibility of the model application in terms of its costs and computational efficiency without compromising the required accuracy of the results.

2.3.2.4 Model calibration and validation

Model calibration and validation are the key stages of any modeling exercise. They are part of the model performance evaluation representing the validity of the modelled processes in a water body. In model calibration, certain parameter values are varied within their reasonable value ranges. The aim of the calibration is to derive a set of parameter values which result in best possible agreement with the measured data. Measured data is usually from the field or the laboratory experiments. Model calibration is necessary as one model can be applied to various water bodies because of its common underlying physical processes. Hence, each model application has its set of parameter values which are either derived from laboratory experiments or are manually set using a trial-and-error approach making it an iterative procedure. While mathematical formulation of the model is related to science, model calibration is commonly referred to as an “art” and depends on the experience of the modeler. Model calibration is then followed by model validation where an independent observed data set is used in comparison with the model results. This dataset is not used in the model set up and the optimized calibrated set of parameters is kept unchanged during validation phase. In most cases, a part of the observed data set is used for calibration while the other part is kept for model validation (James, 2002; Ji, 2008).

A statistical analysis is performed between the observed data and the model results to measure the model performance evaluation. There are several statistical approaches which have been used in the past. These approaches represent model accuracy and are also used as objective functions to derive an optimum set of parameters during calibration. The most common ones are the mean error (ME), mean absolute error (MAE), root-mean-square (RMS) error, relative error (RE), and relative RMS error (RRMSE) (Ji, 2008). Relative root mean square error (RRMSE) is widely used statistical measure to evaluate model performance (Ji, 2008). It is reported as a percent error and is given by

$$RRMSE = \frac{\sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}}}{O_{max} - O_{min}} \times 100\% \tag{1}$$

where O_i and P_i are observed and predicted values respectively and n is the total number of value pairs (Ji, 2008). The numerator in Equation (1) is the root mean square (RMS) error in the same dimensions as the value. Hence, RRMSE is the normalized form of RMS error, by dividing the RMS error with the range of observed data. RRMSE provides a representative measure of model performance for a given output variable. Mean relative RMS error (MRRE) is a measure of overall model performance and is essentially an average value of all the RRMSEs for their respective output variables. It can be used in cases where more than one output variable is simulated such as discharge, sediment rates, and various different pollutants. It also helps in estimating the sensitivity of the model to different parameters (Ji, 2008).

Nash and Sutcliffe efficiency (NSE) is another objective function which has been used in various applications (Bussi et al., 2014). It is primarily used to optimize the set of parameters to quantify the accuracy of the hydrologic models (Bai & Duan, 2014). The NSE ranges from negative infinity to 1 with efficiency of 1 corresponding to a perfect match between the observed and modelled data. An efficiency of 0 represents that the model predictions are similar in accuracy as the mean of the observed data. A negative efficiency value indicates that the mean of the observed data is a better model than the model results. It is given by

$$NSE = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \qquad (2)$$

where $\bar{O}$ is the mean of observed data, O_i and P_i are observed and predicted values respectively and n is the total number of value pairs (Bai & Duan, 2014; Nash & Sutcliffe, 1970).

The study of the Blackstone River by (Ji et al., 2002) used RRMSE for each storm simulation to evaluate the model performance for discharge, sediment, and metal concentrations. MRRE value was also calculated to report the overall sensitivity of the model to variations in input parameters.

The study conducted on Nansha River by (H. Jia et al., 2011) used the monitoring data from a neighboring river for model calibration and validation. This was done because of the unavailability of the long series monitoring data for the Nansha River. Therefore, monthly data from the Changhe River for years 2003 and 2004 was used for calibration and validation. Justification for such an approach is provided in terms of close proximity of Changhe River to Nansha River and similarity in its planning status. This study was conducted for water quality parameters including eutrophication and, therefore, a large parameter set was calibrated. A total of 42 parameters related to water quality simulations were initially obtained from literature. This step was followed by trial-and-error procedure for calibration. Median error was used as the measure of model accuracy. One monitoring point was used to show the calibration and validation results. The average of the median errors during calibration was reported to be 41.34% which is significantly high. Validation statistics show the median error of 29.22%. These results were considered satisfactory by the authors. The model was recommended as a platform for scenario analysis for water pollution control and urban river water environmental management. The reason for such high error values can be the unavailability of the monitoring data for Nansha River itself, as calibration was performed against monitored data for Changhe River.

Chapter 3

Methodology

3.1 Don River Watershed Model

A calibrated hydrologic model for the Don River watershed was provided by the TRCA and was used as a basis for developing an upgraded version of the watershed model. This existing model was developed using PCSWMM modeling software and only routed the overland runoff from subcatchments for a 40-day time period (from June20 to July 30, 2008). This existing model was extended to a time period of 5 months (from April1 to August 31, 2010), and was also parameterized for the TSS and metals modeling capabilities already present in PCSWMM. As a result, the upgraded version of the model was able to simulate TSS and metals loadings from the subcatchments and route them to and through the hydraulic network.

3.1.1 Existing model

The Toronto and Region Conservation Authority (TRCA) provided the calibrated Don River watershed model which was developed in PCSWMM. The model was calibrated for hydrology based on rainfall/runoff simulation from subcatchments. Figure 4 shows the Don River watershed model domain from PCSWMM as provided by TRCA. As can be seen from the figure, the spatial resolution of the model is relatively high, with a total of 475 subcatchments, 2834 conduits, and 2465 junctions in the domain. These subcatchments are assigned to the local rain gauges maintained by TRCA, based on their proximities as can be seen from Figure 4. These rain gauges use tipping buckets, reporting data at a 5-minute frequency, and they are not operated during winter period.

The time span of this existing model is 40 days from June 20 to July 30, 2008. The existing TRCA model for the Don River watershed is only calibrated for flows for the 40 days simulation period and does not contain any pollutant buildup or wash-off simulation. High resolution 5-minute rainfall data from the TRCA rain gauges allow for high temporal discretization of the model. The wet weather time step of 2 minutes is used while for the dry weather, the time step used is 1 hour. A time step of 10 seconds is used for hydraulic routing through the network. The model reports the output at every 5 minutes for a 40 day simulation period.

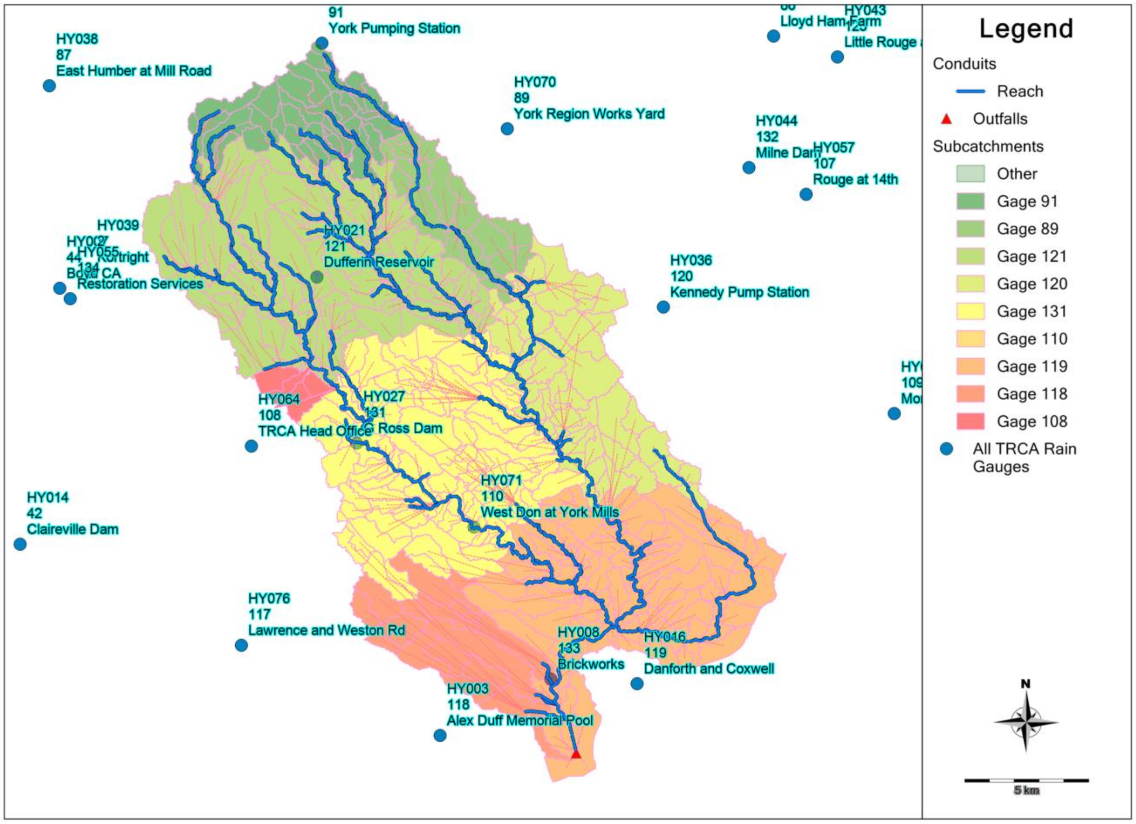

Figure 4: Existing PCSWMM Don River watershed model domain as provided by TRCA

The hydrologic results of the existing TRCA model are shown in Figure 5. The simulated flows at the Todmorden station were reported every 5 minutes. These simulated flows were interpolated to 15-minute intervals to compare the simulated flows with the observed 15-minute flow data. As can be seen from the figure, the model results show a very good agreement with the observed data. A NSE value of 0.873 and RRMSE of 4.59% was reported.

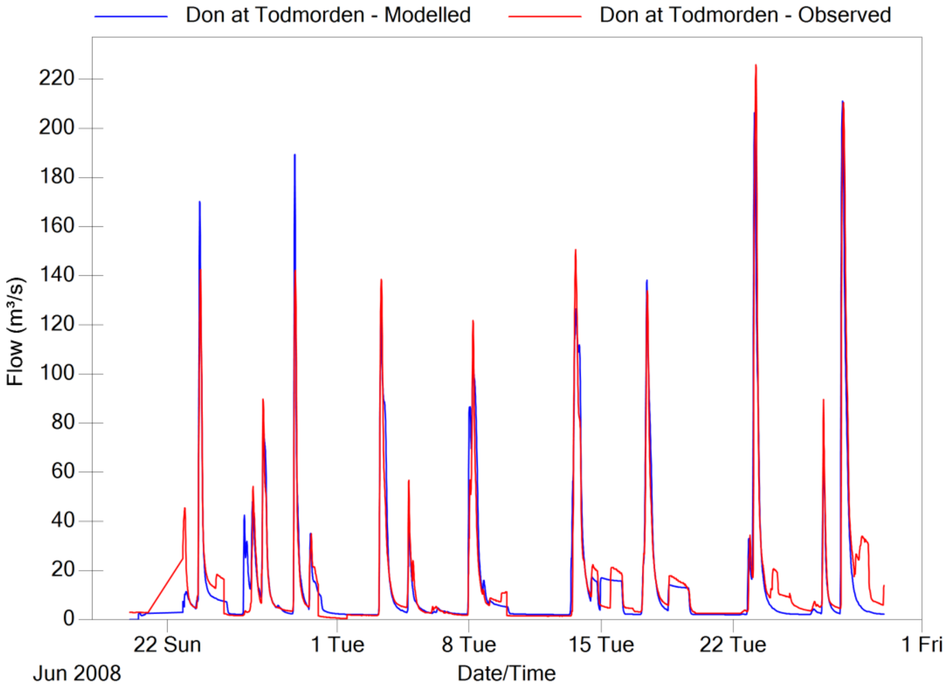

Figure 5: Existing PCSWMM Don River model performance. RRMSE of 4.59%

3.1.2 Simulation of TSS and metal loads

The existing Don River watershed model did not simulate pollutant buildup and wash-off from the subcatchments. Such a capability was required to estimate the sediment loads in the form of TSS along with associated pollutant loads to the study reach. These loads can then be used as non-point source boundary loads in the EFDC model. Therefore, the model was upgraded to include TSS (sand, silt, clay), copper, lead, and zinc simulation using buildup and wash-off functions in PCSWMM. The model was also upgraded to simulate 5 months of rainfall/runoff simulation from April1 to August 31, 2010.

The upgrading process included adding a land use layer to the existing model. The land use layer contained information regarding various types of land uses throughout the watershed for year 2010 including residential, commercial, resource and industrial, government and institutional, parks and recreational and open area. This land use layer, obtained from DMTI Spatial Inc. is shown in Figure 6. It can be seen from the figure that almost the entire watershed has been developed except some areas in the North West part of the watershed.

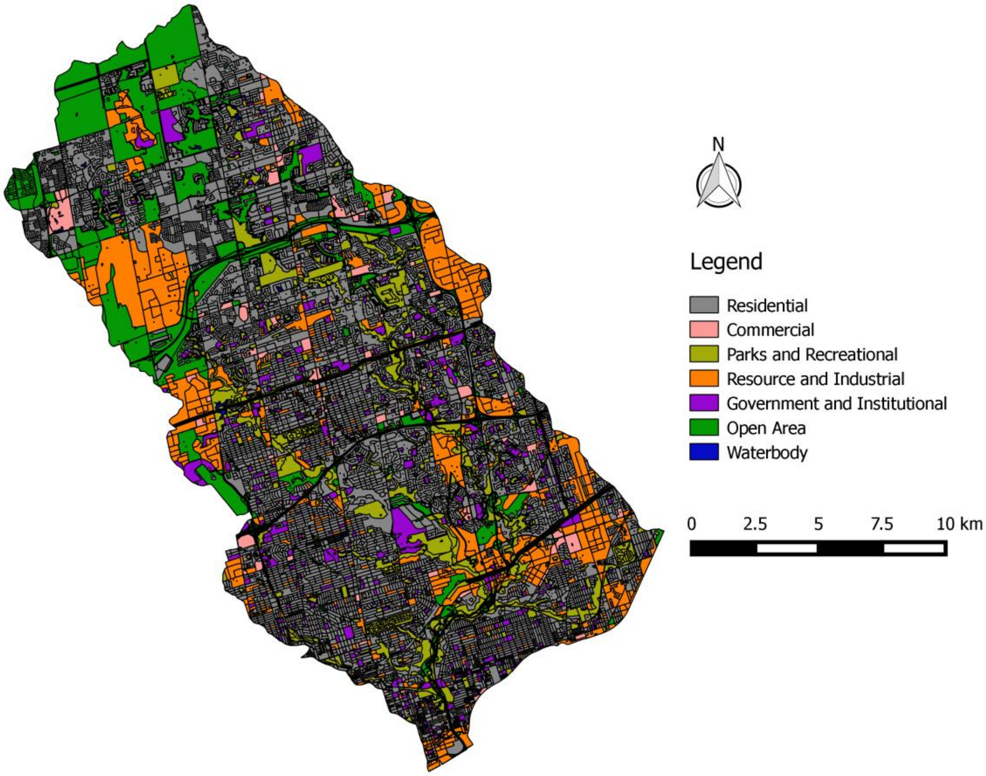

Figure 6: Land use classification of the Don River watershed in 2010. Data based on DMTI CanMap Rail obtained from DMTI Spatial Inc., and mapped using QGIS 2.6

The land use layer was overlaid on the subcatchments layer in PCSWMM and an area-weighting operation was performed using PCSWMM GIS area-weighting tool to assign each subcatchment in the model with various land use areas. Essentially, this operation assigned percentages of various land use categories within each subcatchment in the watershed. Following this process, each land use category was assigned TSS buildup parameters. Exponential buildup equation was used to simulate buildup which is given as

$$B = C_1(1 - e^{-kt}) \qquad (3)$$

where B is the buildup (Kg/ha), C_1 is the maximum buildup possible (Kg/ha), k is the rate constant (1/days) and t is time for buildup (days) during dry periods.

The parameters in Equation (3) are set using values in Table 2. These parameters are derived from an experimental study conducted on a highly urbanized Australian watershed (Hossain et al., 2010).

Table 2: TSS buildup parameters for various land uses in an urbanized watershed (Hossain et al., 2010)

Land Use	Max Buildup, C_1 (Kg/Km^2)	Max Buildup, C_1 (Kg/ha)	Rate Constant, k (1/days)
Residential	1000	10	0.12
Commercial	5300	53	0.222
Open Area	2600	26	0.382
Government and Institutional	5300	53	0.222
Resource and Industrial	5300	53	0.222
Parks and Recreational	2600	26	0.382

The TSS wash-off function was based on event-mean-concentrations (EMCs). The event-mean-concentrations used in this study are the concentrations of TSS that are washed-off from a land use during a storm event. The EMC values were derived from Toronto Wet Weather Flow Management Guidelines shown in Table 3 (City of Toronto, 2006).

Table 3: TSS wash-off concentrations for various land uses in the Don River watershed (City of Toronto, 2006)

Land Use	Concentration (mg/l)
Residential	150
Commercial	120
Open Area	200
Government and Institutional	330
Resource and Industrial	120
Parks and Recreational	130

The washed-off metal concentrations were simulated using PCSWMM pollutant co-fraction approach. This approach involves defining a fraction of the TSS concentration that will control the metal concentration. These co-fractions were calculated from the observed concentrations of TSS and each of the metals (Cu, Pb, Zn) at the Todmorden station. The co-fraction approach used is the simplest way to estimate metal loads using PCSWMM and is also the recommended approach (James et al., 2010), given the general lack of pollutant buildup and wash-off parameters for urbanized catchments. Monthly monitoring data was acquired from TRCA for TSS and metal concentrations for the years 2008 to 2013. Mean of the observed concentrations was calculated for each of the pollutant. The co-fraction of each metal relative to TSS concentration was then calculated by simply dividing the metal concentration by TSS concentration. Metal concentrations are reported in the units of µg/l while TSS concentrations are reported in the units of mg/l. The co-fraction values do not reflect this inconsistency in concentration units because PCSWMM internally converts the co-fraction values to appropriate units. The metal co-fraction values used in upgrading the PCSWMM Don River watershed model are reported in Table 4.

Table 4: Pollutant co-fractions used in PCSWMM derived from 2008-2013 data obtained from TRCA. Unit conversion is handled internally by PCSWMM

Pollutant	Observed Mean Concentration	Observed TSS Mean Concentration	Co-fraction
	(µg/l)	(mg/l)	
Zinc	24.26	55.45	0.438
Copper	7.94	55.45	0.143
Lead	5.06	55.45	0.091

Wash-off loads of sand, silt, and clay components of TSS were simulated by treating these sediment classes as co-fractions of TSS. Annual data for the dredged sediment in Keating Channel was acquired from TRCA for particle size fractions of sand, silt, and clay (Appendix A). Using this data, co-fractions values of 0.12 for clay, 0.25 for silt, and 0.63 for sand were applied.

3.1.3 Extension of model time period

Following the setup of the buildup and wash-off simulation in PCSWMM, the model was allowed to run for a period of 5 months from April 1 2010 to August 31, 2010. The month of April was used as model spin-up period to minimize the impact of initial conditions. The long term 5-minute rainfall data was obtained from TRCA for the rain gauges used in their existing model (Figure 4). This data set was not reliable for winter months and a complete data set could only be observed for the period of May to August for most of the years. For this reason, this time period was considered appropriate for results comparison and analysis. The upgraded model used a wet time step of 5 minutes and a dry time step of 30 minutes reporting results every 15 minutes. A hydraulic routing time step of 8 seconds was used to run the simulation. A smaller hydraulic routing time step increases the numerical stability and computational efficiency of the model as lesser number of numerical iterations are required to converge to a solution.

The results from this upgraded and extended watershed model are saved in SWMM binary output file and GIS shapefiles for subcatchments, conduits, and junctions generated by PCSWMM. These files are then used to extract the required data for set up of the EFDC hydrodynamic, sediment transport, and metals fate and transport model. A tool called the SWMM to EFDC model setup tool (STEMS) is developed to achieve this linkage, which uses these output files from PCSWMM.

3.2 SWMM to EFDC Model Setup Tool (STEMS)

SWMM to EFDC model setup tool (STEMS) was developed in MATLAB® R2014b to efficiently setup the EFDC hydrodynamic model using the hydrologic results and geospatial layers of PCSWMM. All the GIS layers that are used in STEMS are provided from PCSWMM after running the PCSWMM model. The tool consists of 17 functions in total with 4 core functions and a main executable file that form the bases of the tool. These 4 core functions call other utility functions repeatedly during the run to perform necessary data operations. The schematic of STEMS is shown in Figure 7.

The main input to the STEMS tool is the conduit shapefile of the river of interest. If branches or tributaries are also being modelled, then the user must provide the individual conduits shapefiles of these tributaries connected to the main river. In order for STEMS to work properly, the tributaries must only be connected to the main river and not another tributary connected to the main river. Moreover, each continuous river reach should be provided as a single shapefile. Other shapefile layers such as subcatchments, junctions, and conduits of the entire model domain from PCSWMM are also provided as input to STEMS. Finally, STEMS prompts for the PCSWMM output binary file which is used for extracting data for boundary conditions definition in EFDC.

STEMS uses the data from the input shapefiles and generates the 1D cartesian grid for EFDC model setup. The grid contains data defining the geometry of each cell using the conduit shapefiles provided from PCSWMM. Each conduit is treated as a cell in EFDC grid. However, this EFDC grid is independent of the geographic coordinates. In order to initialize this grid, STEMS prompts for initial grid coordinates which can be arbitrary or kept at default values that STEMS uses. Once the user has provided all the required inputs, STEMS will execute displaying the summary of inputs in the command window and save the outputs in the user specified directory.

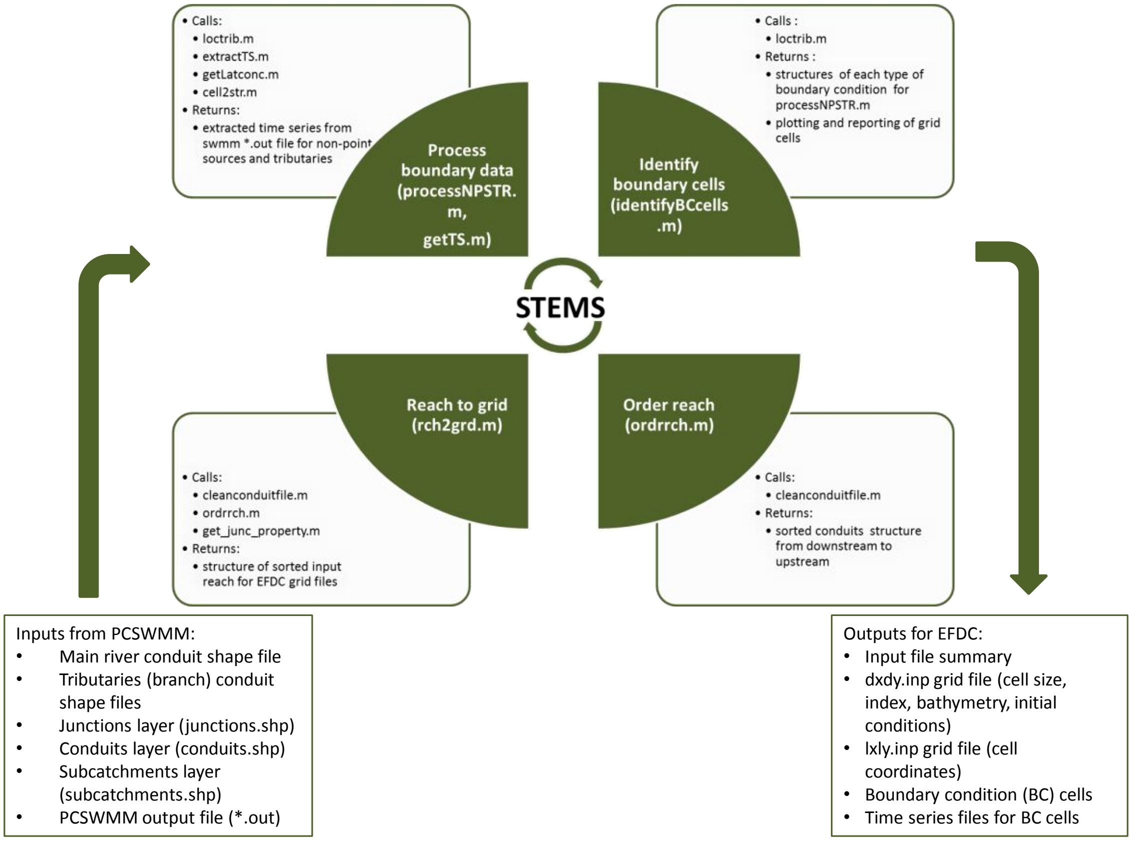

Figure 7: SWMM to EFDC model setup tool (STEMS) schematic

3.2.1 Order reach (ordrrch.m)

The main purpose of the order reach core function is to sort the individual conduits in the input conduit shapefile in a continuous downstream to upstream direction. The shapefile is read and stored in a MATLAB® structure array. This function is necessary because the input conduit shapefiles from PCSWMM may not always be in a definite continuous order. If such is the case, data interpretation and manipulation from this structure array becomes illogical for further processing. Therefore, this function uses the logical sequence of adjoining junctions of each conduit in the input shapefile to sort the individual conduits in a downstream to upstream direction.

This function named ‘ordrrch.m’ calls another utility function called ‘cleanconduitfile.m’. The main purpose of this utility function is to remove any duplicate conduits which exist as parallel conduits to represent various custom cross-sections at different inlet and outlet elevations. The utility function only keeps the conduits which are at the same invert elevation as its adjoining junctions and removes the others. This preserves the actual bed bathymetry of the river as used in PCSWMM and does not affect the results for EFDC setup.

3.2.2 Reach to grid (rch2grd.m)

The main purpose of the reach to grid core function is to generate the sorted structure array with the fields required for the EFDC grid files. This function converts the sorted conduit shapefile into a structure array containing fields of cartesian coordinates and other cell geometry parameters for each conduit. The cell lengths and widths are obtained from the information contained in the conduit shapefile. The widths are top widths or maximum spreads of the irregular conduits. For custom conduits, average of the conduit width upstream and downstream of the custom conduit is used. The average width approach is used because PCSWMM does not provide a field for a representative width of a custom cross-section in its conduit shapefile. The function accepts grid initialization parameters as input arguments which are provided by the main STEMS program. This function operates on each input conduit shapefile to return a structure array for EFDC grid which is further used to identify the boundary condition cells.

This core function named ‘rch2grd.m’ calls two utility functions ‘cleanconduitfile.m’ and ‘get_junc_property.m’ along with the core function ‘ordrrch.m’. The purpose of the utility function ‘cleanconduitfile.m’ and core function ‘ordrrch.m’ is explained in the previous section. The utility function ‘get_junc_property.m’ returns the required property of the specified junction. It is used to get the junction properties such as elevations and total inflows to the junctions. The conduit slopes and their adjoining junction elevations are used to calculate the elevation at the center of the conduit. This center elevation is assigned as the elevation of the grid cell in EFDC. This elevation information along with lateral and total inflows to the cell is used to populate fields in the returned structure array which is used for EFDC grid definition and boundary condition cell identification.

3.2.3 Identify boundary cells (identifyBCcells.m)

The main purpose of the identify boundary cells core function is to identify the boundary condition cells in the global grid structure array. The global grid structure array is the grid structure created after combining individual structure arrays returned from rch2grd.m for each input shapefile. In essence, the global grid structure contains the grid data for the whole EFDC model domain. The function plots the entire grid as well as the boundary cells and saves the figure in the working

MATLAB® directory. It also returns the identified boundary cells in separate tables which are further written to MS Excel files in the specified directory.

The main types of boundary conditions identified are flow boundary condition cells which consist of tributary inflows and runoff from subcatchments (non-point sources). These boundary cells are associated with flow type boundary condition receiving water flux and pollutant loads. Other boundary conditions include the upstream boundary cells and the downstream boundary cell. Conduits with custom cross-sections are also identified and labelled on the grid plotted by this function. However, these custom cross-sections are not relevant in EFDC and are labelled for visual purposes.

This core function calls the utility function named 'loctrib.m' that locates the cells in the grid which have tributaries inflows. This utility function is useful in locating the tributaries that are not modelled by the user, and hence, not included in the grid based on the modeling requirements. These 'invisible' tributaries, although not modelled, provide external inflows to the modelled reach as point sources, and therefore, should be accounted for. The utility function uses the conduits shapefile for the entire domain from PCSWMM to search for the tributaries which are connected to the study reach but not modelled. The most downstream conduit information for the 'invisible' tributary connecting to the main river channel is stored in a separate structure array for that location. These structure arrays at different tributary locations are stored in a cell array which is the returned output of the 'loctrib.m' utility function.

3.2.4 Process boundary data (processNPSTR.m, getTS.m)

Two functions that process the boundary condition data are described in this section. The core function named 'processNPSTR' is specifically written for flow type boundary condition cells (where flow from tributaries and subcatchments come in), whereas, the function 'getTS.m' is for upstream and downstream boundary condition cells. Both these core functions take the structure array for boundary condition cells as input arguments and returns the time series data for each of the boundary cells in a cell array of tables. This output is further used to create text files containing time series data, which are saved in the specified directory.

The core function 'processNPSTR.m' uses four utility functions (Figure 7). The utility function named 'loctrib.m' is explained in the previous section. The utility function named 'extractTS.m' extracts the time series for a given junction, conduit, or subcatchment for a given parameter. It runs a script called ‘swmmtoolbox0.5.5’ (Cera, 2013) written in Python language, which must be preinstalled onto the system. This Python script reads the SWMM binary output file and returns the time series results of a given parameter for a given junction, conduit, or subcatchment. The utility function ‘extractTS.m’ takes the junction, conduit, or subcatchment name as input argument along with the parameter for which the data is required. This parameter can be flow or name of any pollutant modelled. It then runs the Python script and returns the extracted data as a time series table. The data from this time series table is then further processed by the core functions.

The utility function named ‘getLatconc.m’ returns the lateral concentrations of modelled pollutants into the junction from their respective subcatchments. It uses the entire subcatchments shapefile layer from PCSWMM to search for those subcatchments whose outlet junction identifies the flow type boundary condition cell. It then extracts the runoff concentration time series data by calling the ‘extractTS.m’ utility function for those subcatchments.

The core function named ‘processNPSTR.m’ provides resultant flows and loads for the flow type boundary cells. This essentially means that if a boundary cell receives flow from both the subcatchment runoff and tributaries which are not modelled, then the function will sum the flows of the two sources to provide a net flow into that boundary cell. If the boundary cell receives flow from only one of the sources, then the flow from that source will be assigned to that boundary cell.

Similarly, for the pollutant concentrations, the function processes the data such that it assigns flow-weighted concentration if a cell receives pollutant loads from one or more than one subcatchment and/or tributaries which are not modelled. Hence, this ensures that the flow type boundary cells only represent the external resultant loads in defining the boundary conditions in EFDC model.

The core function named ‘getTS.m’ omits the above mentioned processing to obtain resultant loads. This is because ‘getTS.m’, when applied to upstream cell, simply uses the ‘extractTS.m’ function to get the total loadings into the domain from that cell. The same core function is used for downstream boundary to get the water level time series from PCSWMM output file.

A utility function named ‘cell2str.m’ is written to access the contents of the MATLAB cell arrays containing string type variables. This function is written for easy handling of structure arrays with string type fields. It simply returns the contents of a cell containing a string type variable.

These core functions take the most computation time in STEMS run due to repeated data extraction from the SWMM binary output file. The run time depends on the size of the output file and the number of pollutants for which the time series data is required. Once the data has been extracted and processed, STEMS will save the time series data in a text file for each pollutant or parameter in the specified directory.

3.3 STEMS Outputs

A copy of the upgraded and extended PCSWMM model for the Don River watershed was saved to modify the study reach. The irregular cross-sections of the study reach were truncated to their active banks. This operation was performed to obtain the active top width of the irregular cross-section. A field in the conduit shapefile layer called “maximum spread” reports the maximum top width of the irregular conduit during a complete simulation. To make use of this field for the purpose of obtaining representative top widths of the conduits, truncation of the study reach is necessary. Once the cross-sections of the study reach are truncated, the model is run to get the updated conduit GIS shapefile layer. The conduit shapefile for the study reach is then saved as a separate shapefile. This conduit shapefile for the study reach is used in STEMS to get the appropriate cell widths for EFDC grid. (See section 3.2.2)

The unmodified study reach version of the model was run to obtain the SWMM output file. This file was used to extract the external boundary condition data using STEMS for EFDC model setup. It is to be noted, however, that the SWMM output file from the modified study reach version of the model will provide the same results as the unmodified version. This is because SWMM output file is used to extract the external loads, which are not affected by truncating the cross-sections of the study reach. The only purpose of truncating the cross-sections of the study reach is to obtain conduit top widths for assigning appropriate cell widths for EFDC grid.

The major outputs of STEMS are the generic nodal grid definition files named ‘dxdy.inp’ and ‘lxly.inp’. The file ‘dxdy.inp’ contains the cell geometry and the initial bathymetry information whereas file ‘lxly.inp’ contains the cell center coordinates information. EFDC Explorer uses these two files to setup the grid and generate a new model. Once the grid is setup in EFDC Explorer, the initial water level and bathymetry can be easily manipulated if required. The plot of the input shapefiles and the resulting grid is also provided by STEMS. This can be used to verify the results when creating the grid in EFDC Explorer using the ‘dxdy.inp’ and ‘lxly.inp’ grid files. This STEMS output can be seen in Figure 8. It can be noted that the 1D EFDC grid is independent of the geographic coordinates used in the input shapefiles. Moreover, the grid shows various types of boundary cells including the non-point source (NPS) cells and tributary cells. NPS cells and tributary cells are categorized as flow type boundary cells in EFDC. Custom cross-section cells are also shown for visual purposes.

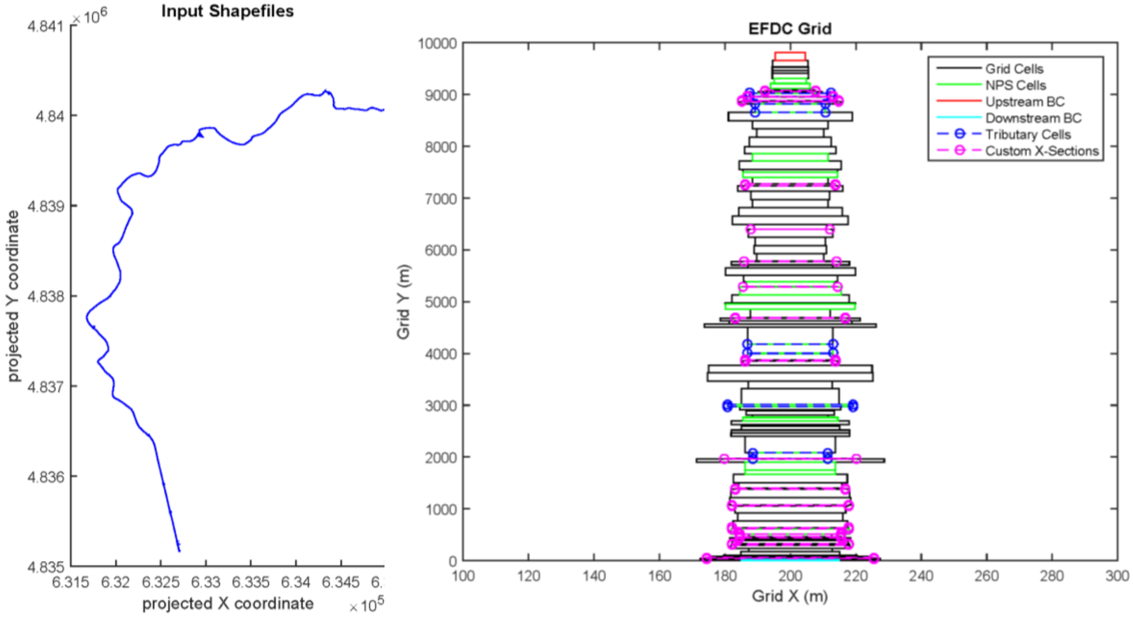

Figure 8: Conversion of input reach shapefile (study reach) to 1D EFDC grid using STEMS tool

The STEMS tool also outputs tables of boundary cells, which are saved as MS Excel files in the specified directory. Table 5 shows this output for flow type boundary cells. It contains the location information of each conduit that has external flow associated with it. This table was used to define the flow type boundary cells after generating the grid in EFDC Explorer. Similarly, the upstream and downstream boundary cells are also reported to easily verify and define these types of boundaries in EFDC Explorer.

The STEMS tool also generates text files containing time series data for all the boundary cells and saves them in the specified directory. A text file is created containing time series data of all the external flows to the flow type boundary cells. Other text files are created depending on the number of pollutants for which the boundary time series data is required. Each text file contains flow-weighted concentration time series for all the flow type boundary cells for each type of pollutant. The format of these text files is such that each column represents data for a boundary cell using proper headers. The format is made compatible for easy import and setup of the boundary conditions in EFDC Explorer.

Table 5: Flow type boundary condition cell information table provided by STEMS tool. Inlet node ID and outlet node ID defines the location of the conduit in the PCSWMM model, whereas, cell I and J indices and their center coordinates define the location of the cell representing that conduit in the EFDC grid

PCSWMM			EFDC			
Conduit ID	**Inlet node ID**	**Outlet node ID**	**Cell I index**	**Cell J index**	**Cell X coordinate**	**Cell Y coordinate**
C44.3	44.3	J48.8	5	51	200	4088.81
CJ41.009	44.1	J41.007	5	96	200	8993.72
CJ43.015	J43.015	J43.014	5	100	200	9159.33
CJ43.016	J43.016	J43.015	5	101	200	9259.33
CJ44.05	J44.05	J44.03	5	63	200	5340.36
CJ44.29_2	J6	J44.28	5	82	200	7443.96
CJ44.31	J44.31	J44.30	5	85	200	7781.62
CJ44.37	44.2	J44.36	5	91	200	8731.71
CJ48.46	J48.46	J48.44	5	16	200	565.65
CJ48.61	J48.61	J48.60	5	27	200	1706.15
CJ48.62	J48.62	J48.61	5	28	200	1823.65
CJ48.65	J47.0	J48.64	5	31	200	2029.04
CJ48.676	J48.678	J48.675	5	38	200	2730.01
CJ48.71	48.1	J48.70	5	43	200	2994.78
CJ48.88	J48.88	J48.87	5	58	200	4904.20
CJ48.92	J44.02	J48.91	5	61	200	5204.01

3.4 EFDC Model Setup

The model development in EFDC Explorer 7.2 was achieved through a step-by-step process. The first step in the development of the model was grid generation. This step was followed by setting up the boundary condition cells in the grid and linking them to the boundary time series data. Once the grid and boundary condition cells were initialized, hydrodynamic simulation was performed. Hydrodynamic simulation was calibrated before proceeding with the sediment transport simulation with an active sediment bed. Following the calibration of the sediment transport simulation, metals were introduced into the model and calibrated against observed concentrations. These steps of model development are explained in the same order in the following sections.

The model used a warm-up period of 43 days from April 1 to May 13, 2010 for sediment transport and metals simulation before model data comparison was conducted from May 13 to August 31, 2010. The warm-up simulation was conducted to minimize the impact of the initial conditions. However, given that the study reach has many external inflows and is subject to flash floods, the impact of initial conditions is not expected to be significant.

3.4.1 Grid initialization

The first step in developing the EFDC model was developed by creating a 1D grid of the study reach using the dxdy.inp and lxly.inp generic grid nodal files created by STEMS tool. The bathymetric information was retrieved from PCSWMM model using the STEMS tool and is contained in the dxdy.inp file (see section 3.2.2). The generated grid and bathymetry of the study reach is shown in Figure 9. Note that the grid structure and geometry can be verified using the grid plotted by STEMS shown in Figure 8.

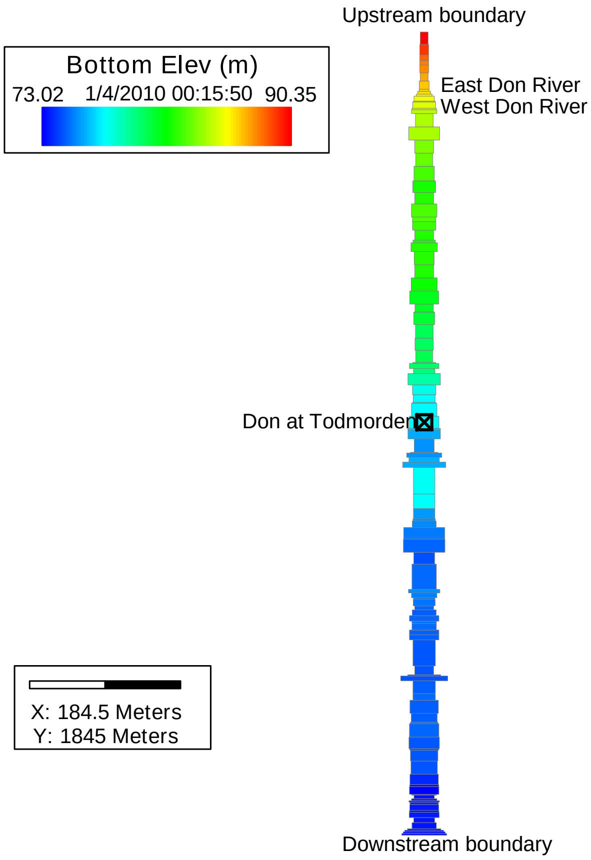

Figure 9: EFDC model domain and initial bathymetry. Mapped using EFDC Explorer 7.2

The initial bed elevation ranges from 73.02 m above sea level (masl) at the mouth of the reach draining into the Keating Channel (downstream boundary) to 90.35 masl at Taylor Creek South (upstream boundary). The longitudinal profile of the study reach shown in Figure 10 provides the details of bed elevation. The bed slope is relatively shallower just upstream of the Todmorden station and at the downstream section where it drains into the Keating Channel. The initial water surface elevation shown in the figure is obtained after a 122 day warm-up hydraulic simulation from May to August 2010.

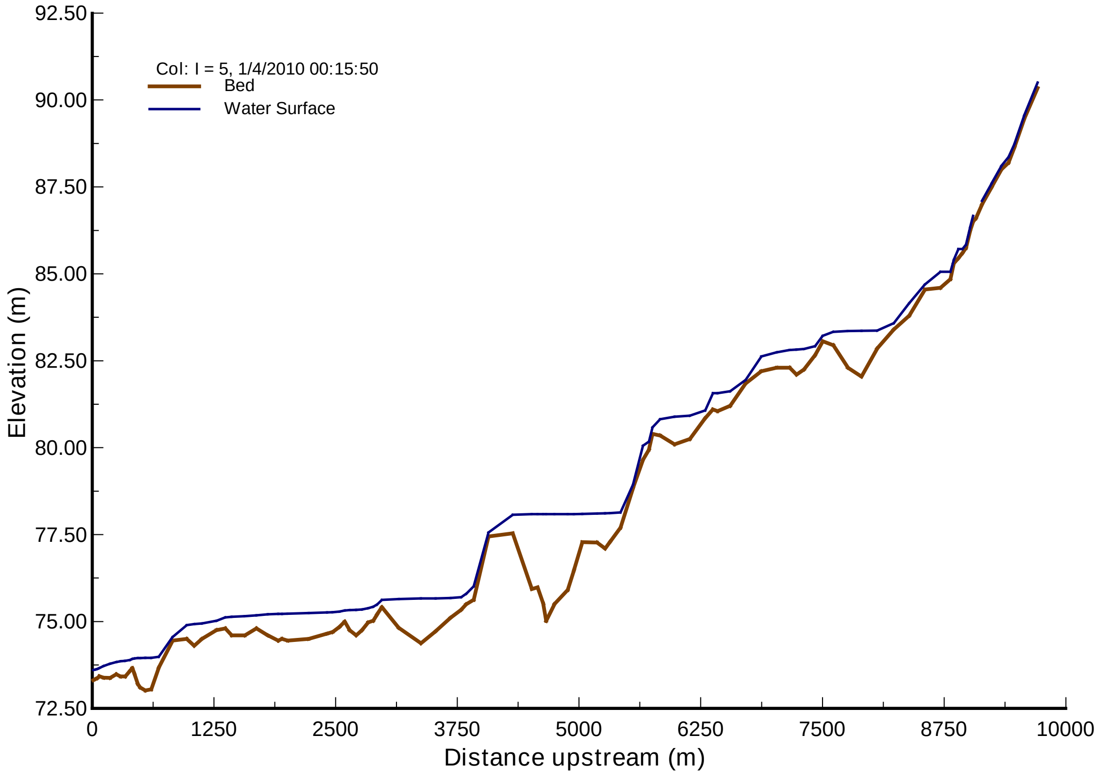

Figure 10: Lower Don River initial longitudinal profile (discharge value of 1.36m^3/s at Todmorden station). Plotted using EFDC Explorer 7.2

The grid statistics summary is shown in Table 6. There are a total of 105 active cells covering an area of 28.2 ha. Cell widths range from 9.3 m at upstream section to 57.4 m at the mouth of the study reach where it drains into the Keating Channel. The average cell width is 30.0 m. The total length of the study reach is 9.81 Km with cell lengths ranging from 4.5 m to 325.4 m with an average length of 93.2 m.

Table 6: EFDC general grid statistics

Grid Properties	Values
Total number of active cells	105
Total active cell area (ha)	28.2
Minimum cell width (m)	9.3
Maximum cell width (m)	57.4
Average cell width (m)	30.0
Minimum cell length (m)	4.5
Maximum cell length (m)	325.4
Average cell length (m)	93.2

The variable time step option was used for EFDC simulations, which is handled internally by EFDC. This ensured numerical stability of the hydraulic model for the given spatial discretization. The sediment transport simulation used twice the time step of the hydraulic model. This is justified by the fact that sediment processes are generally slow allowing for higher time steps without compromising the numerical stability of the results.

3.4.2 Boundary conditions

Figure 11 provides information for the grid structure along with locations of the boundary cells assigned to the grid. There are a total of 17 flow type boundary cells along with an upstream boundary cell and a downstream open boundary. These boundary cells are reported as part of the STEMS output (Table 5), using data files from PCSWMM hydrologic model results. The location of the boundary cells in the EFDC grid can be easily assigned using this information.

Once these boundary cells were defined, time series data for flow was imported from a text file generated by STEMS tool. Flow time series for each boundary cell in the text file was verified and linked to its respective boundary cell. The same procedure was followed for importing text files containing concentration time series data for pollutants. These time series included concentration data for sand, silt, and clay fractions along with metal concentrations. This process was performed in a progressive manner; sediment boundary data was imported first and results were calibrated followed by each of the metals.

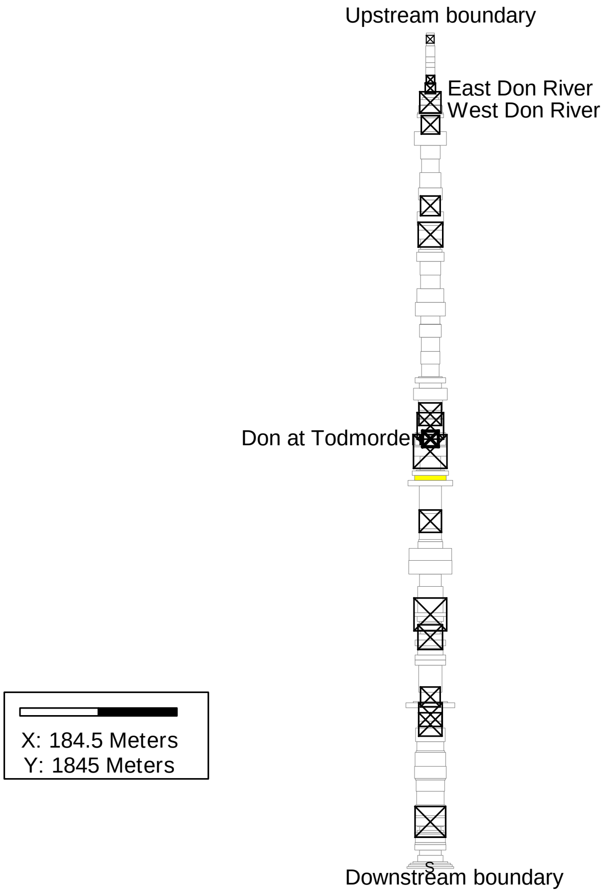

Figure 11: EFDC model boundary cells. Mapped using EFDC Explorer 7.2

3.4.3 Hydrodynamic and sediment transport configuration

Hydrodynamic model was configured after setting up the flow boundary condition data for the model. The roughness height was the only calibration parameter in the hydraulic model and a value of 0.08m, provided satisfactory results. This roughness height is within the range of 0.01m to 0.1m recommended by the expert user community of the EFDC model.

Sediment transport simulations were performed with an active sediment bed after hydraulic results were considered satisfactory. Due to lack of sediment core data for the study reach, sediment bed was initialized using a 5 cm uniform bed thickness. This initial bed thickness is consistent with the Blackstone River study (Ji et al., 2002). Using the particle size fractions in the dredged sediment of Keating Channel obtained from TRCA data (see Appendix A), sediment bed was initialized to contain 12% clay, 25% silt and 63% clay fractions.

The porosity of the sediment bed was calculated by using typical porosity values (Geotechdata.info, 2013) of each of the soil types or size classes (Appendix A). These values along with the mass fractions of these classes provided a weighted porosity value of 0.44. Specific gravity of the sediments was fixed at 2.65. Bulk density of the sediment bed and dry sediment concentration was then calculated internally by EFDC using these fixed parameters. Table 7 provides the values for these fixed parameters used to configure the sediment bed.

Table 7: Sediment bed properties used for Lower Don River in EFDC

Sediment bed parameter	Value
Porosity	0.44
Bulk density (Kg/m^3)	1921
Dry sediment concentration (Kg/m^3)	1480

Silt and clay were modelled as cohesive sediments using particle diameter of 30µm and 10µm respectively, whereas sand was modelled as non-cohesive sediment with a particle diameter of 410µm. Table 8 and Table 9 provide the values of parameters used for each sediment class. Silt and clay use the same values of parameters as cohesive sediments. All the parameters in Table 8 are calibration parameters and were calibrated using trial-and-error approach to provide the closest results to the observed data. Typical range of critical deposition shear stress for cohesive sediments range from 0.10 to 0.25 N/m^2 and critical erosion shear stress is typically taken to be 1.2 times the critical deposition shear stress (Ji et al., 2002). Settling velocity of 0.001 m/s is also consistent with the values reported for cohesive sediments in various case studies by (Ji, 2008). A parameter called the reference surface erosion rate is used by EFDC to define the bed surface erosion process for cohesive sediments. It is a value multiplied with the normalized excess shear stress (a fraction) to calculate bed erosion rate. Reference erosion rate of 0.09 g/m^2/s was calibrated to provide good agreement of TSS concentrations with the observed data.

Table 8: Calibrated parameters for cohesive sediments used in EFDC for Lower Don River

Parameter	Clay(10µm)	Silt(30µm)
Settling velocity (m/s)	0.001	0.001
Critical deposition shear stress (N/m^2)	0.16	0.16
Critical erosion shear stress (N/m^2)	0.192	0.192
Reference erosion rate (g/m^2/s)	0.09	0.09

Parameters for non-cohesive sand particles were different from that of cohesive sediments. The parameters were based on the concept of critical Shield’s stress for incipient motion. These parameters are dictated by grain size of the sand particles. The sand particle diameter was calibrated to represent typical sand grain size, and a value of 410 µm provided good agreement with the observed data. This diameter value was used internally by EFDC, applying the Van Rijn formulations to compute critical shields stress, critical velocity, and settling velocity of the non-cohesive particles.

Table 9: Parameters for non-cohesive sediment used in EFDC for Lower Don River

Parameter	Sand
Diameter (µm) (calibrated)	410
Critical Shield's Stress	0.032
Critical stress (N/m^2)	0.21
Critical velocity (m/s)	0.014
Settling velocity (m/s)	0.061

Sediment transport simulation was performed with an active bed allowing bed elevation changes during simulation. Results for total TSS concentrations at Todmorden were compared with observed data for calibration. After the results were considered satisfactory, metals simulation was configured and activated.

3.4.4 Metals parameterization and calibration

Boundary condition cells were linked with concentration time series data which was imported from text files created by STEMS tool for each metal. Each metal was configured using a simple sorption model in EFDC Explorer 7.2. Table 10 provides the summary of the partition coefficients for sediment bed and water column used in the model. These partition coefficients are all calibration parameters and their values were calibrated using trial-and-error approach in EFDC. A report by United States Environmental Protection Agency (US EPA) providing experimental results for partition coefficients of various metals in water, sediment, and waste was used as a guide to calibrate the partition coefficients in this study (Allison & Allison, 2005).

The initial sediment bed concentration assigned for copper was 74 mg/Kg, while for lead and zinc the initial bed concentrations were set at 30mg/Kg and 148mg/Kg. These initial bed concentrations were assigned based on an interpolated general trend of these metal concentrations in the dredged sediment of the Keating Channel over the past years. These sediment bed initial concentrations were subjected to a warm-up simulation of 43 days, although, longer warm-up time periods, based on the available data resources, are preferred for sediments and metals because of their relatively slower response. (Bussi et al., 2014; Ji et al., 2002). For fast river systems with many external inflows and floods, the system tends towards equilibrium relatively faster, and therefore, a relatively shorter warm-up time period (e.g. 60 days) is sufficient (Ji, 2008). However, this conservative approach of assigning initial sediment bed metal concentrations close to the observed trends ensured that the system attained equilibrium within the warm-up time period of 43 days, thereby minimizing the impact of such initial conditions. The initial water column concentration of each metal was assigned a value of 0µg/l, which was not based on actual conditions, but water column responses tend towards equilibrium relatively faster. Hence, the warm-up time period of 43 days was deemed sufficient for the adjustment of these initial water column concentrations. The diffusion coefficient was kept at a typical value of 1E-09 m^2/s for water column and sediment bed.

After the toxic module of EFDC Explorer 7.2 was configured and activated using the above parameters for metals, the model was allowed to run. EFDC runs the metals simulation parallel to the sediment transport simulation. In fact, the metals simulation module of EFDC cannot be activated without activating the sediment transport module; metals transport processes are associated with sediment transport. After the run was completed, the results for total metal concentrations at Todmorden station were compared with the observed data.

Table 10: Partition coefficients used in EFDC for contaminant modeling in the Lower Don River

Partition coefficients, K_d for water column (l/mg)			
	Clay	**Silt**	**Sand**
Copper	0.001	0.001	0.0003
Lead	0.003	0.003	0
Zinc	0.1	0.1	0.0003
Partition coefficients, K_d for sediment bed (l/mg)			
Copper	0.03	0.03	0.03
Lead	0.03	0.03	0.03
Zinc	0.013	0.013	0.013

Chapter 4

Results

4.1 Hydrologic Results of the Upgraded PCSWMM Model

The hydrologic results of the upgraded PCSWMM model are shown in Figure 12. The time period used to report the results was from May 1, 2010 to August 31 2010 with April time period used for warm-up simulation. The results of this upgraded model were reported every 15 minutes, while the observed flow data obtained from Environment Canada Water Survey reported daily average discharge. This observed flow data was used because a higher resolution flow data was not available from the TRCA flow gauge at Todmorden for the modeling time period. Therefore, simulated flows were interpolated to represent daily average flows in order to compare with the observed daily flows at Todmorden.

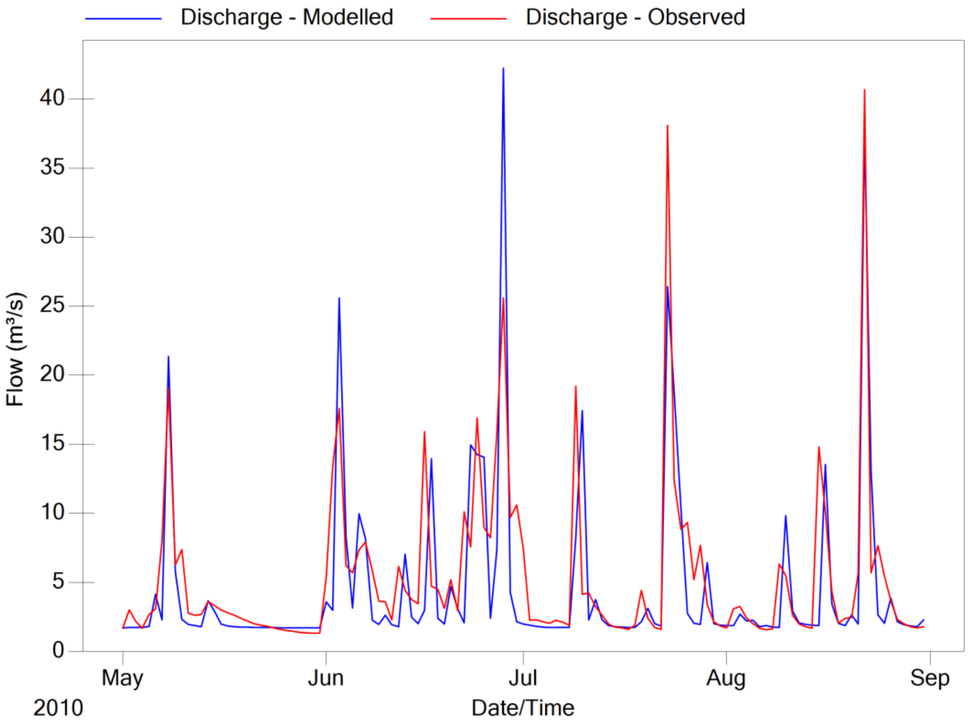

Figure 12: Observed vs PCSWMM modelled hydrograph at Todmorden. RRMSE of 10.63%

The simulated results show a very good agreement with the observed data as can be seen in Figure 12; the RRMSE of 10.63 % was reported. All the peak flows were reasonably captured and the timing of the peaks was also in good agreement along with the base flow. It is to be noted that the hydrologic component of the existing PCSWMM model provided by TRCA was not modified. Only the time span of the simulation was increased for a different year to perform a long term simulation.

4.2 Sediments and Metals Results of the Upgraded PCSWMM Model

Figure 13 through Figure 16 show the comparison of the upgraded PCSWMM model results for sediments and metals with the observed concentrations at Todmorden station. The results were reported every 15 minutes of simulation. The water samples from Todmorden station were collected monthly under the Provincial Water Quality Monitoring Network (PWQMN) and the concentration data was provided by TRCA. Hence, the observed concentration data for the period of interest from May to August 2010 had four samples, and therefore, four observed data points. The water sample result of June 26 represented a storm event.

The modelled results of TSS concentrations shown in Figure 13 depict large discrepancy when compared to the observed data. The modelled peak concentrations are significantly lower than the observed peak concentration of 794 mg/l observed for a storm event on June 26. Moreover, the base flow concentrations are also highly over estimated. This discrepancy in results was expected since PCSWMM is only capable of routing the washed-off TSS from the subcatchments through the hydraulic network without applying any in-stream processes. The only purpose of upgrading the PCSWMM model to simulate TSS and metals was to obtain the wash-off loads from subcatchments to define boundary loads in EFDC as non-point source loads.

Similar trend in modelled concentration and observed data was seen for copper and zinc as shown in Figure 14 and Figure 16. The modelled peak concentrations were significantly underestimated when compared to the concentration values of 52.6µg/l and 156µg/l for copper and zinc respectively, representing a storm event on June 26. The base flow concentrations were close to the observed concentration for copper but slightly overestimated for zinc. Due to limitations of PCSWMM in-stream pollutant modeling capabilities, these results were not in agreement with the actual concentration trend at Todmorden. Only the simulated wash-off loads from subcatchments were used as boundary loads in EFDC as mentioned above.

Results for lead concentrations compared with the observed data at Todmorden station can be seen in Figure 15. Lead concentrations are very low relative to other metals. The modelled peaks are within the observed concentrations range.

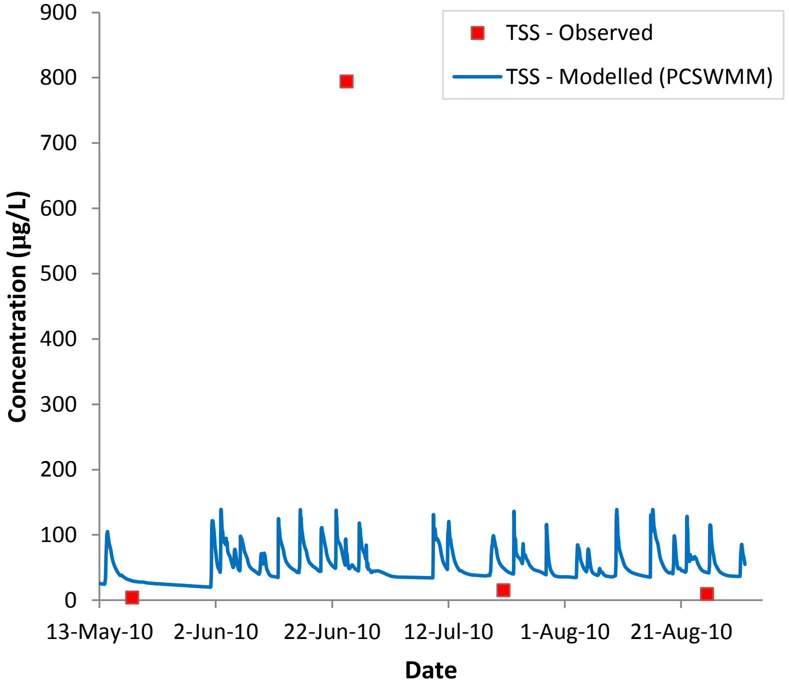

Figure 13: Observed vs PCSWMM modelled TSS concentration at Todmorden

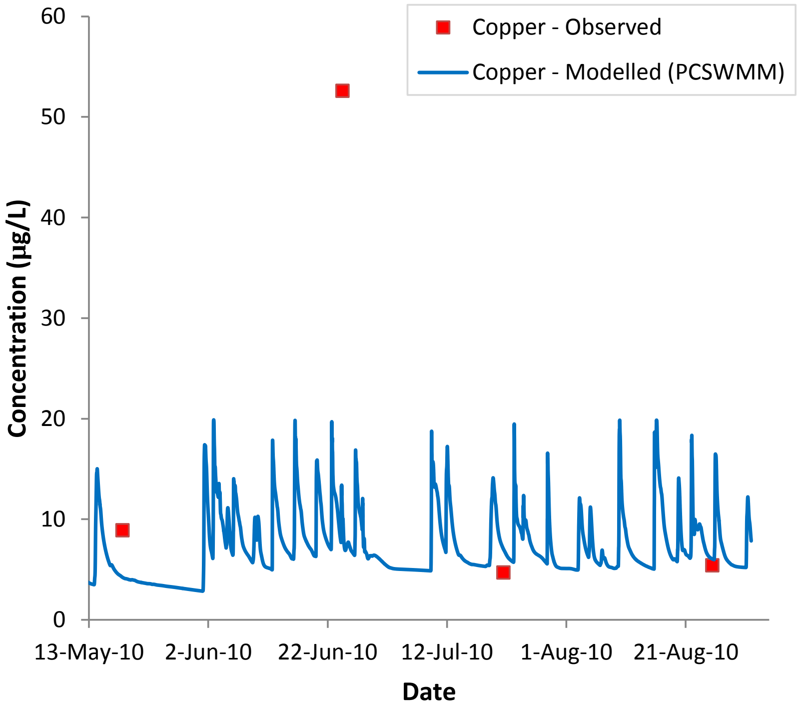

Figure 14: Observed vs PCSWMM modelled copper concentration at Todmorden

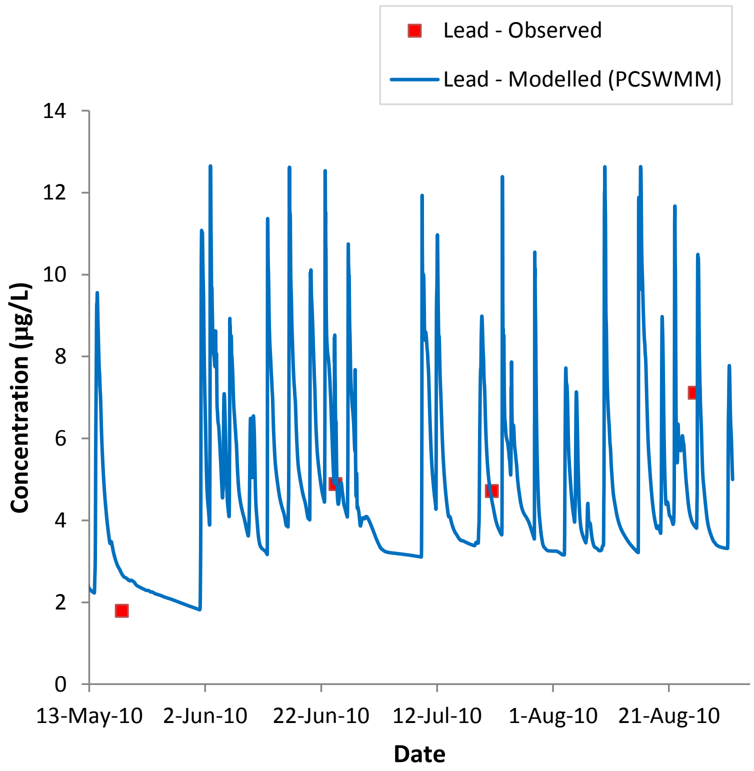

Figure 15: Observed vs PCSWMM modelled lead concentration at Todmorden

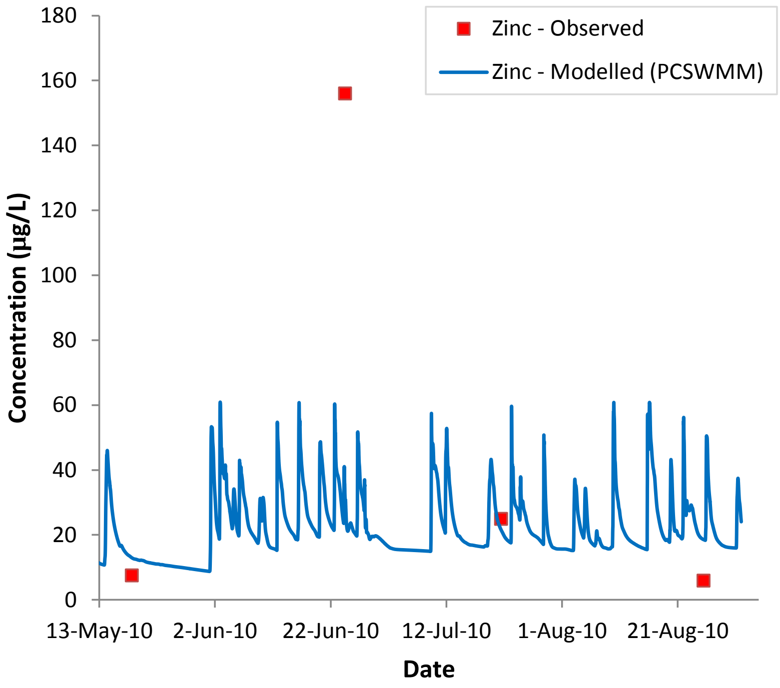

Figure 16: Observed vs PCSWMM modelled zinc concentration at Todmorden

4.3 EFDC Hydrologic Results

Runoff results of the upgraded PCSWMM model were used to set up the non-point source boundary flows in EFDC model. The hydrologic results from the EFDC model are shown in Figure 17. The model data comparison was conducted from May1, 2010 to August 31, 2010 at the Todmorden station. The simulated results from EFDC were reported every 15 minutes and were converted to daily average flows for comparison with the observed Environment Canada daily average flows.

The results were in good agreement with the observed flow hydrographs reporting a RRMSE of 11.98%. The timing and magnitude of the peaks and base flow corresponded with the observed data.

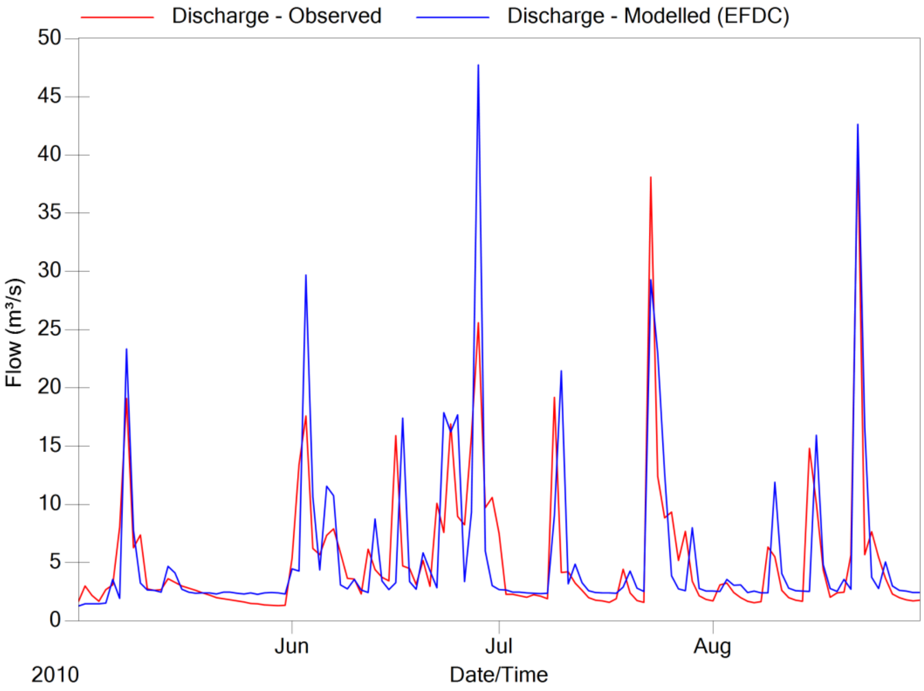

Figure 17: Observed vs EFDC modelled hydrograph at Todmorden. RRMSE 11.98%

4.4 EFDC Sediments and Metals Results

The results of TSS and total metals concentration simulated by EFDC are shown in Figure 18 through Figure 21. The results were reported every 15 minutes of simulation and the model data comparison was conducted from May 13, 2010 to August 31, 2010 at the Todmorden station.

As can be seen from Figure 18, modelled TSS concentrations showed very good agreement with the observed data points. The observed TSS concentration of 794mg/l representing a storm event on June 26 was reasonably captured by the modelled concentration. Moreover, the modelled peak concentrations corresponded with the peak flows shown in Figure 17. However, it is to be noted that concentration data was reported at a temporal resolution of 15 minutes, whereas flow hydrograph in Figure 17 is a result of interpolation to daily average flows. Furthermore, the base flow TSS concentrations predicted by EFDC for other months were also in good agreement with the observed data. These results can be compared with the results of the upgraded PCSWMM model shown in Figure 13.Unlike the results of the PCSWMM model, EFDC simulation provided a more reliable prediction of the peak concentrations representing storm events along with the base flow concentrations.

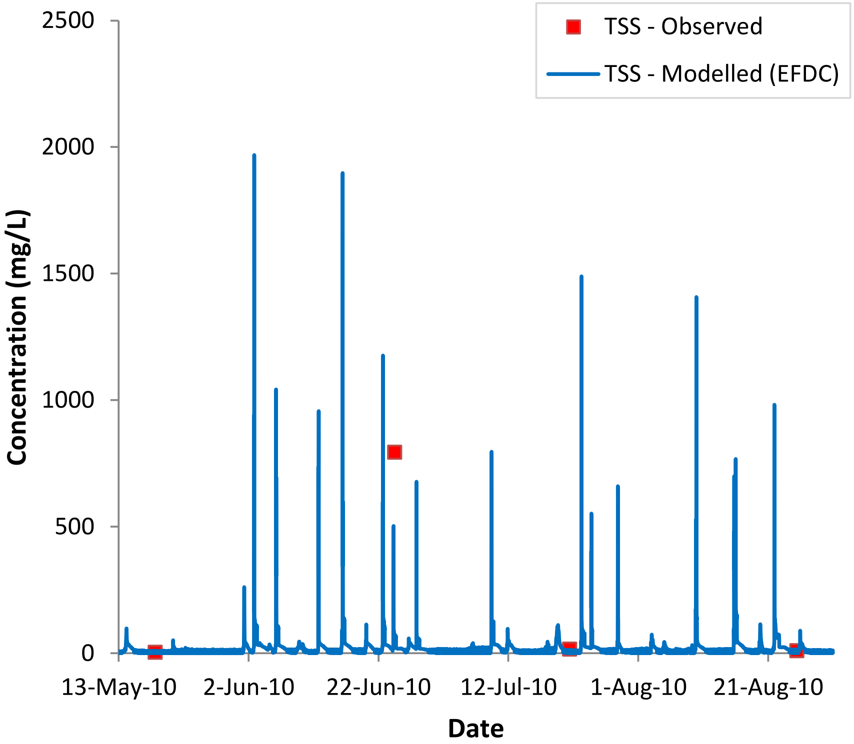

Figure 18: Observed vs EFDC modelled TSS concentration at Todmorden

The results for copper concentrations modelled by EFDC are shown in Figure 19. It can be seen from the figure that modelled copper concentrations show very good agreement with the observed data. The peak concentration value of 52.6µg/l from June 26 storm event was well captured. Moreover, the base flow concentrations of copper from other months were also well predicted compared to the observed concentration data points. These results when compared to the results from the PCSWMM model shown in Figure 14 are more representative of the actual conditions in the study reach.

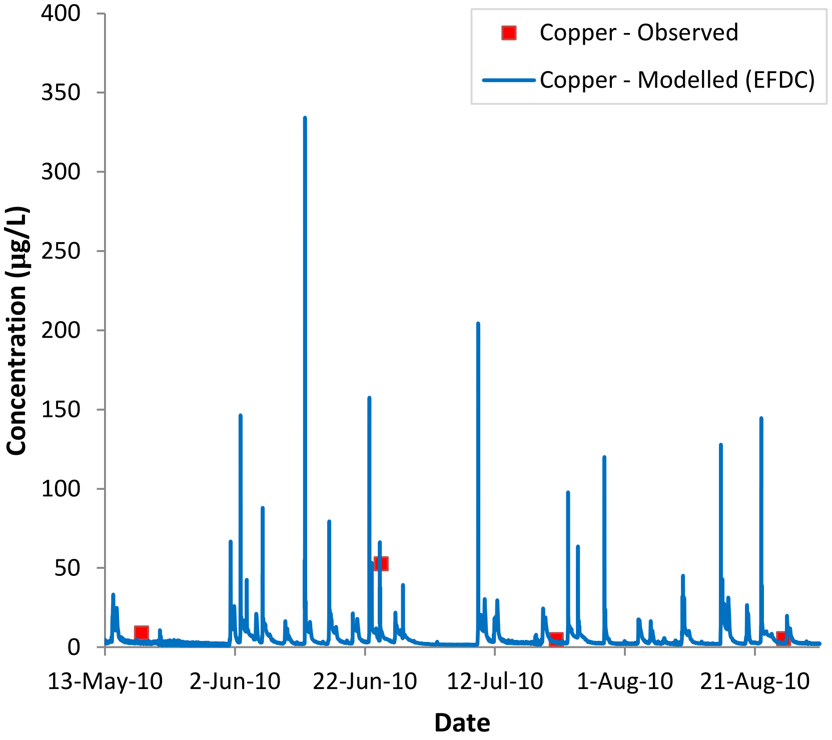

Figure 19: Observed vs EFDC modelled copper concentration at Todmorden

The model data comparison of total lead concentrations is shown in Figure 20. The results were considered to be in good agreement with the observed concentrations. The peak concentrations reflect the storm events with maximum concentration not exceeding 80µg/l. The results reported by EFDC were considered representative of the actual conditions of the study reach.

The results for zinc concentrations shown in Figure 21 were also found to be in good agreement with the observed data. The observed concentration from the storm of June 26 was accurately captured along with the base flow concentrations from other months, unlike the PCSWMM model results shown in Figure 16. These results further enforced the reliability of EFDC results as representative of the actual conditions in the study reach.

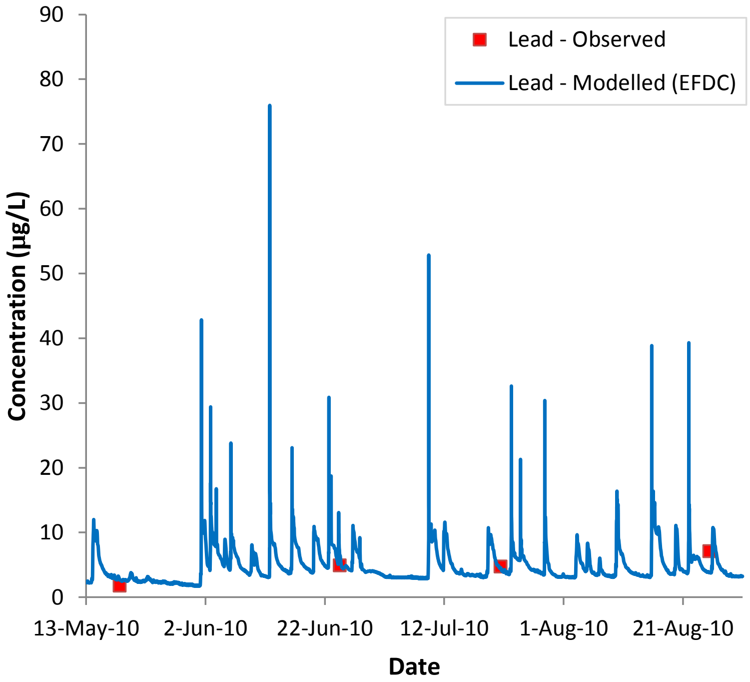

Figure 20: Observed vs EFDC modelled lead concentration at Todmorden

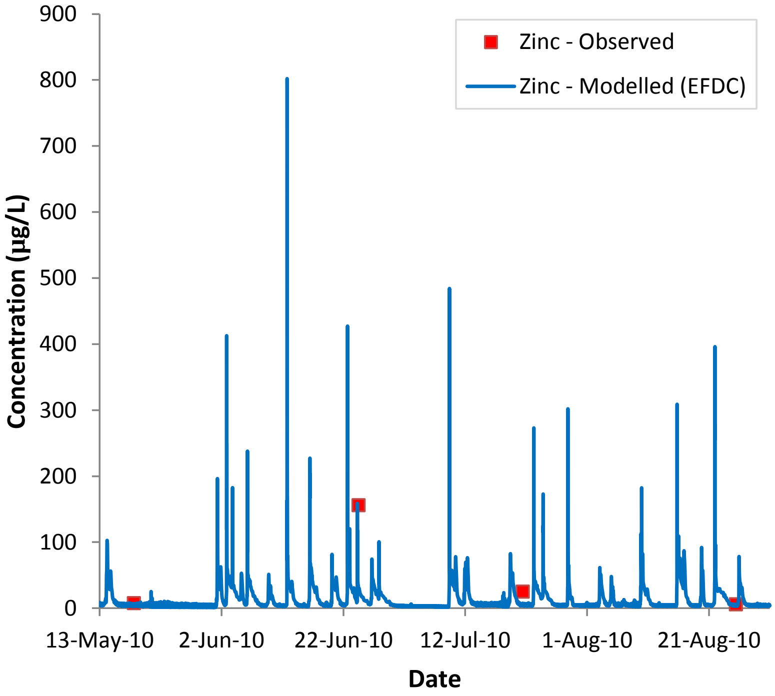

Figure 21: Observed vs EFDC modelled zinc concentration at Todmorden

Chapter 5

Analysis and Discussion

The calibrated EFDC model explained in Chapter 4 provides reasonable and representative estimates of sediment and metals concentration at the Todmorden monitoring site for May to August 2010 time period. Therefore, further analysis was conducted and performance of the two models, PCSWMM and EFDC, was compared and analyzed.

The hydrodynamic results of the two models were similar and did not show any discrepancies. As can be seen from Figure 22, the hydrographs obtained from PCSWMM and EFDC at Todmorden station show the exact same shape, although the EFDC hydrograph show a relatively minor positive offset compared to PCSWMM modelled hydrograph. This offset may be justified by the fact that the two models incorporate a different grid structure. The EFDC model uses a rectilinear cartesian grid, whereas the PCSWMM model uses the cross-section data to define its conduit links. The RRMSE was reported to be only 3.68% between the two hydrographs which furthers confirms the water flux agreement between the two models.

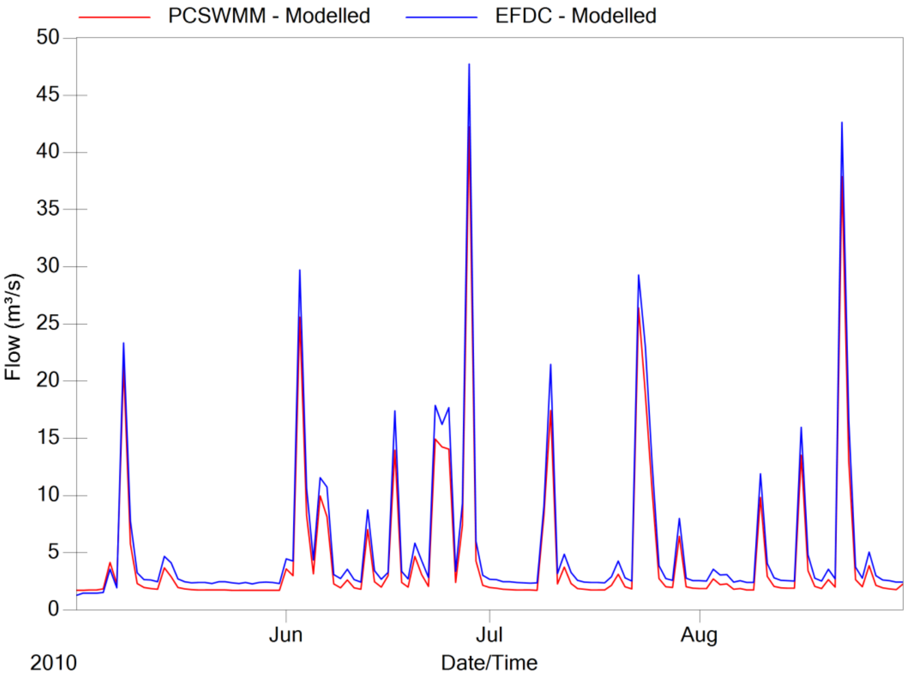

Figure 22: Comparison between EFDC and PCSWMM modelled hydrographs at Todmorden. RRMSE 3.68%

Velocity results of the two models at the Todmorden monitoring station were also analyzed. As can be seen from Figure 23, the results show a positive agreement in terms of correlation of the velocities with RRMSE of 3.57% and R^2 value of 0.89. This further endorses that the hydraulic response of the two models is similar. A few points representing the lower limit of the velocity range (up to 0.4m/s) show a relatively higher modelled velocity by PCSWMM. This scatter in the comparison of the lower velocity values may be explained by the small difference in the baseflow obtained from the two models (Figure 22), which may be due to the different 1D grid structure of the models as mentioned above. However, at lower levels of flow and velocity, the sediment and metal results are not affected, so this small difference is not expected to impact the overall results.

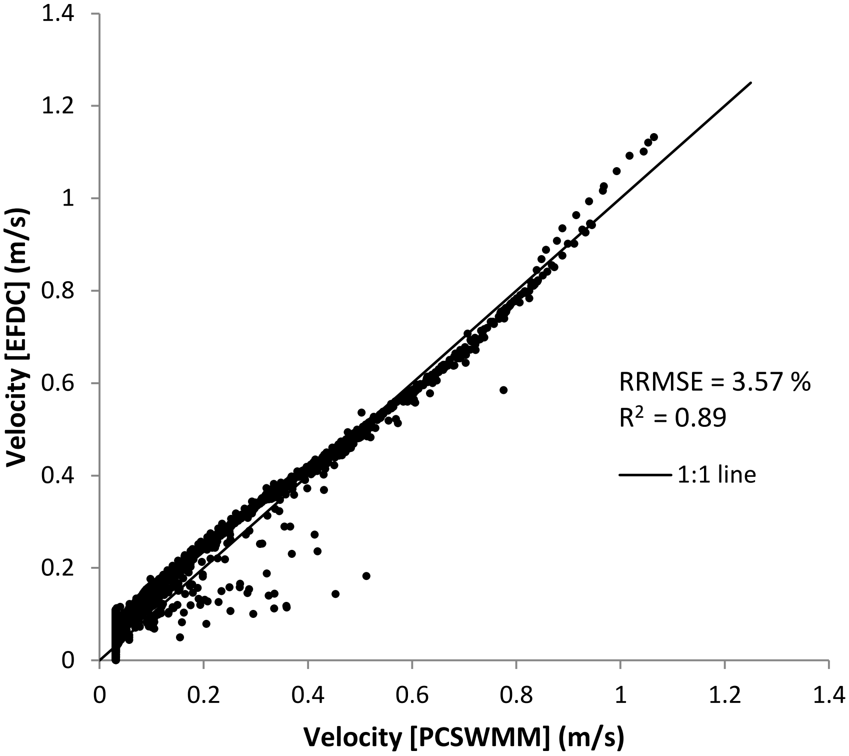

Figure 23: PCSWMM and EFDC modelled velocity correlation at Todmorden

From such high correlation between the hydraulic results of the two models, it can be inferred that the hydraulic results of the EFDC model are dependent on the inflow boundary conditions provided by the PCSWMM hydrologic model. Any change in these boundary conditions will obviously be reflected in the EFDC modelled hydrograph. Since the two models have high correlation in their hydraulic response, any change in PCSWMM overland runoff will be reflected in the EFDC hydraulic results. This further shows high sensitivity of EFDC hydrodynamic results to the provided flow boundary conditions.

The sediment and metal concentration results of the PCSWMM and EFDC model show a significant difference. This result is expected since PCSWMM hydrologic model assumes plug flow routing for its pollutants. This essentially means that the pollutants are undergoing advection only through a series of well-mixed control volumes. Such a routing assumption may not be valid for complex transport processes which involve erosion and deposition of sediments based on bed shear stresses and sorption mechanism associated with metal contaminants. However, PCSWMM model is capable of estimating overland pollutant runoff based on buildup/wash-off model and co-fraction approach discussed in section 3.1.2. These estimates were considered satisfactory based on the provided parameters for the purpose of this research.

EFDC model results for sediments and metals show a valid representation of the actual physical processes controlling their transport. The results of EFDC model can be compared to PCSWMM model from the figures provided in section 4.2 and section 4.4. From these figures, it can be observed that the results of the EFDC model are much more reliable and representative of the actual in-stream conditions. This is expected since EFDC has the capability to simulate in-stream sediment transport processes for individual sediment size classes which include deposition and erosion process based on simulated bed shear stresses. Moreover, the metals fate and transport involves sorption of these metals to individual sediment size classes along with diffusion processes between sediment bed and water column interface. Therefore, such detailed modeling of in-stream processes as in EFDC will produce reliable results using the same boundary loads which were generated through PCSWMM. This further reinforces the importance of modeling the detailed in-stream physical processes for reliable representation of the natural conditions of a river, rather than using simple routing assumptions which may be invalid.

It is to be noted that both PCSWMM and EFDC models are compared using the same boundary loads from overland runoff for their in-stream hydraulic simulations. The baseflow concentration of TSS modelled by PCSWMM is significantly higher at approximately 55mg/l (Figure 13), compared to the value modelled by EFDC at approximately 4 mg/l (Figure 18). Since both the models are provided with the same loadings for their hydraulic routing, this difference in TSS baseflow concentration explains the deposition of TSS which is represented in the EFDC simulation. This deposited sediment is resuspended during flood events providing a source of TSS from the stream bed. The initial sediment amount on the bed also accounts for the additional source of TSS during a high flood event. Although TSS buildup and wash-off calibration is recommended to better represent the Don River watershed specific parameters, the observed peak concentration value of TSS at approximately 800mg/l cannot be captured using the PCSWMM model even after calibration of these parameters (Figure 13). This peak is observed during a flood event causing resuspension of sediments, which is not represented in PCSWMM. Therefore, from the baseflow and peak concentration analysis, the comparison of the two models in terms of their capabilities to represent in-stream processes is further justified.

Further analysis was conducted for the water column concentration of TSS and each of the metals at the Todmorden monitoring station. Observed concentration data from monthly or bi-monthly samples obtained from TRCA and the corresponding daily flow data from Environment Canada was used to plot concentration versus flow scatter plots as shown in Figure 24 to Figure 27. The data used was from year 2008 to 2013. These observed sediment and metals rating plots were compared with the modelled results. Two interpretations of the modelled results were used. The first comparison is made with the modelled results reported at 15-minute frequency, and the second comparison is made with the daily averages derived from the results reported at 15-minute frequency. As can be seen from the figures, the modelled results lie within the general population of the observed concentrations and flows. The modelled daily averages show good agreement with the suggested trend during low flow events for TSS and metals. For high flow events, modelled daily averages start to deviate from the suggested trend. This is because the instantaneous high concentration corresponding to a high flow value is not adequately represented in daily average value. For this reason, modelled results at 15-minute frequency are also plotted to represent instantaneous high concentrations. Only the values within the observed concentration and flow data limits are reported for better representation. The instantaneous concentrations at high flows show wide range of concentrations for TSS and each of the metals. This analysis shows that most of the TSS and associated metals are transported in relatively shorter bursts within longer flood durations. This further leads to show the need for high frequency monitoring and modelling of sediment and metal transport in an urban river system. Comparing the metals concentrations versus flow trends, it can be noted from Figure 26 that lead shows the lowest range of concentrations among the metals with zinc being the most abundant.

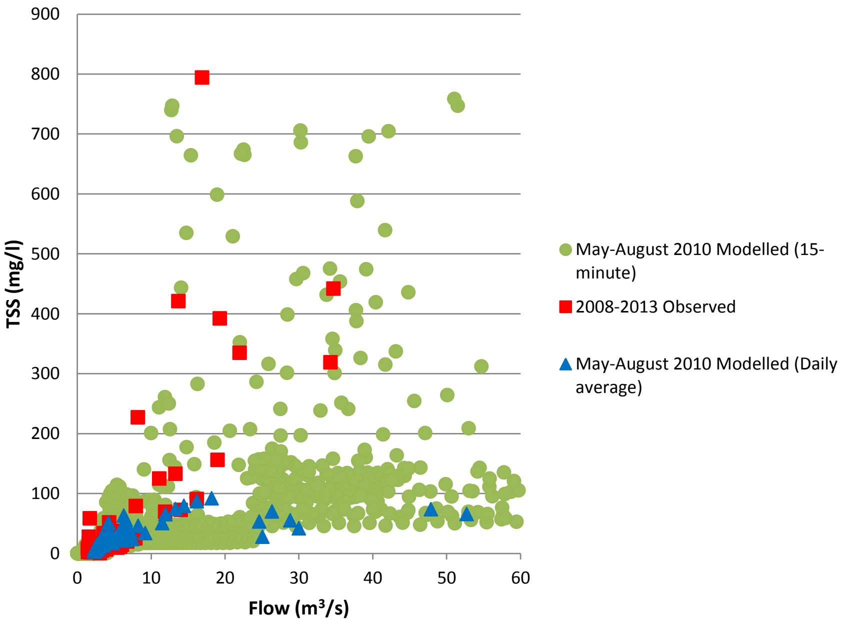

Figure 24: TSS concentration vs flow comparison at Todmorden site for observed and modelled results. Observed concentration data obtained from TRCA Regional Watershed Monitoring Program

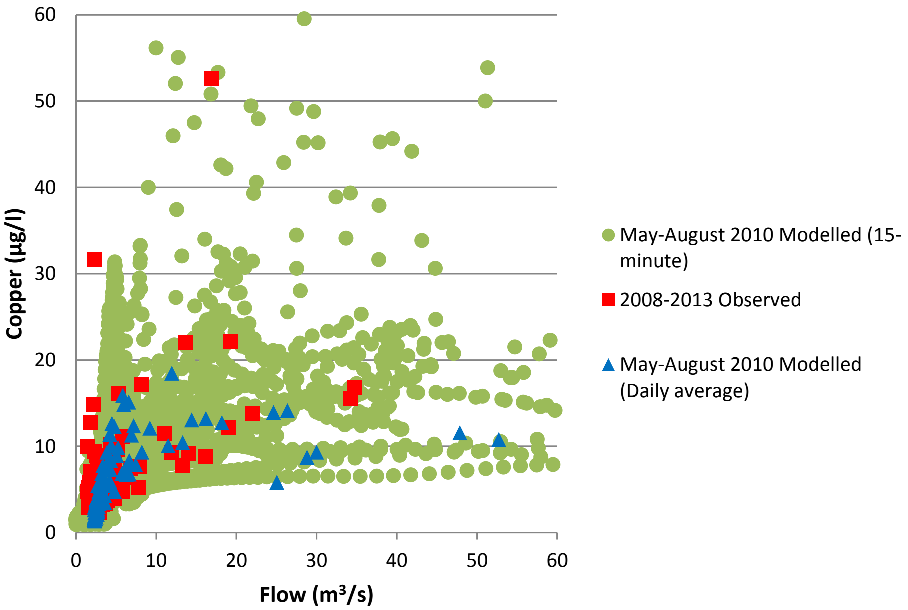

Figure 25: Copper concentration vs flow comparison at Todmorden site for observed and modelled results. Observed concentration data obtained from TRCA Regional Watershed Monitoring Program

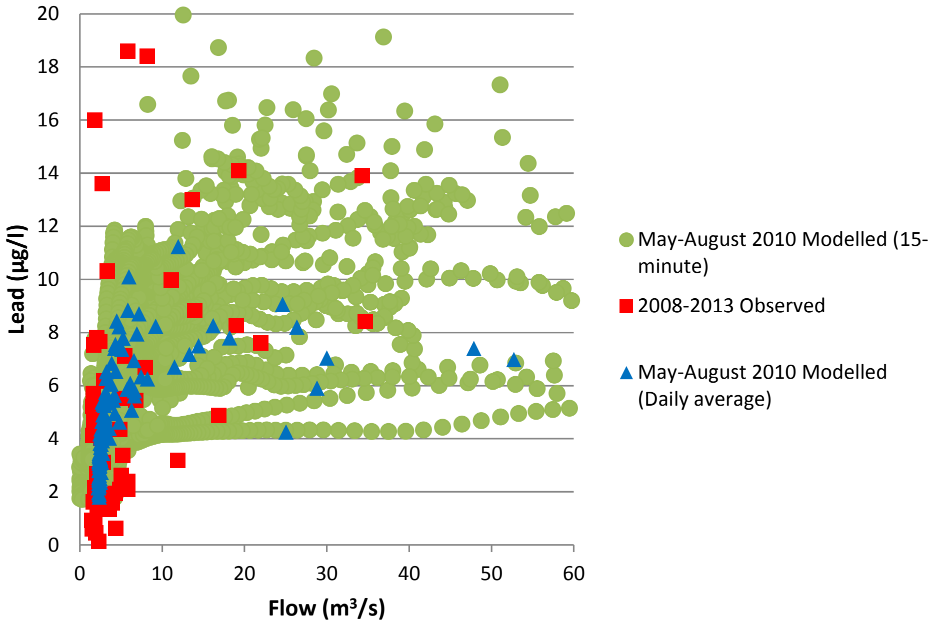

Figure 26: Lead concentration vs flow comparison at Todmorden site for observed and modelled results. Observed concentration data obtained from TRCA Regional Watershed Monitoring Program

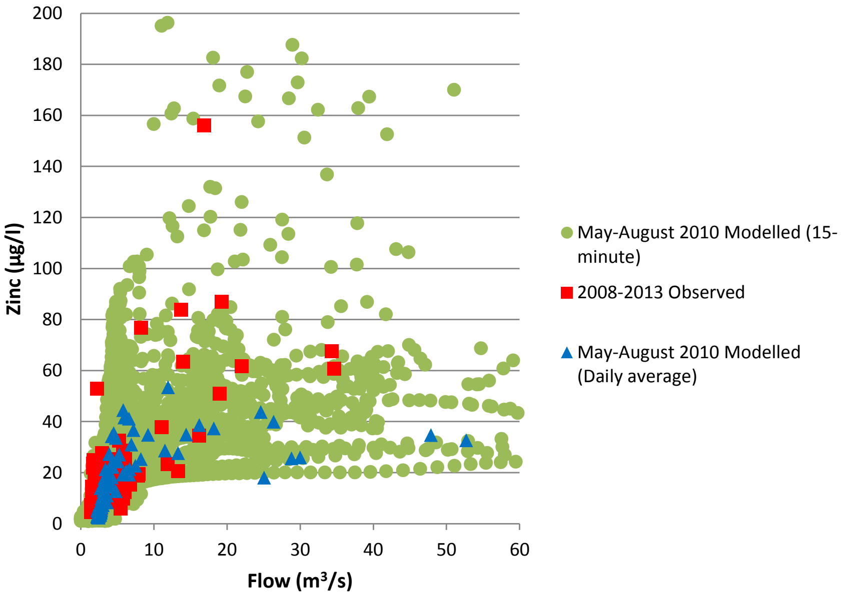

Figure 27: Zinc concentration vs flow comparison at Todmorden site for observed and modelled results. Observed concentration data obtained from TRCA Regional Watershed Monitoring Program

Furthermore, the sediment bed metal concentrations were analyzed to further verify the reliability of the model for better understanding of the dynamics of the lower Don River. The simulated sediment bed data for metal concentrations at the mouth of the study reach at the Keating Channel was analyzed. These concentrations were reported at the end of the simulation period. Sediment bed concentration was reported to be 46.7mg/Kg for copper, 18.7mg/Kg for lead, and 93.3mg/Kg for zinc. The results were compared with the observed long term trend of sediment bed metal concentrations obtained from TRCA from year 1987 to 2014. The results were also compared with the results of the study conducted by (Louie, 2014) who measured sediment bed metal concentration values in April 2014 in the lower Don River. These results can be seen in Figure 28 to Figure 30. The modelled concentration value of each of the three metals in the sediment bed at the Keating Channel agrees well with the observed data and lies within the observed trend. These results show that the developed EFDC model for the lower Don River can be used to predict sediment bed metals concentration into the Keating Channel with reliability.

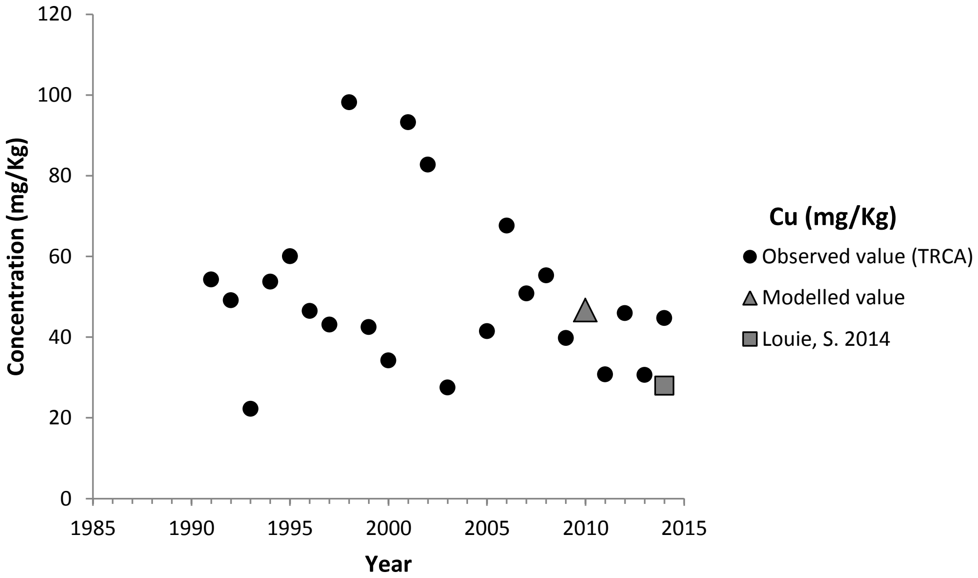

Figure 28: Copper concentration in the dredged sediment at Keating Channel. 1991 to 2014 data obtained from TRCA

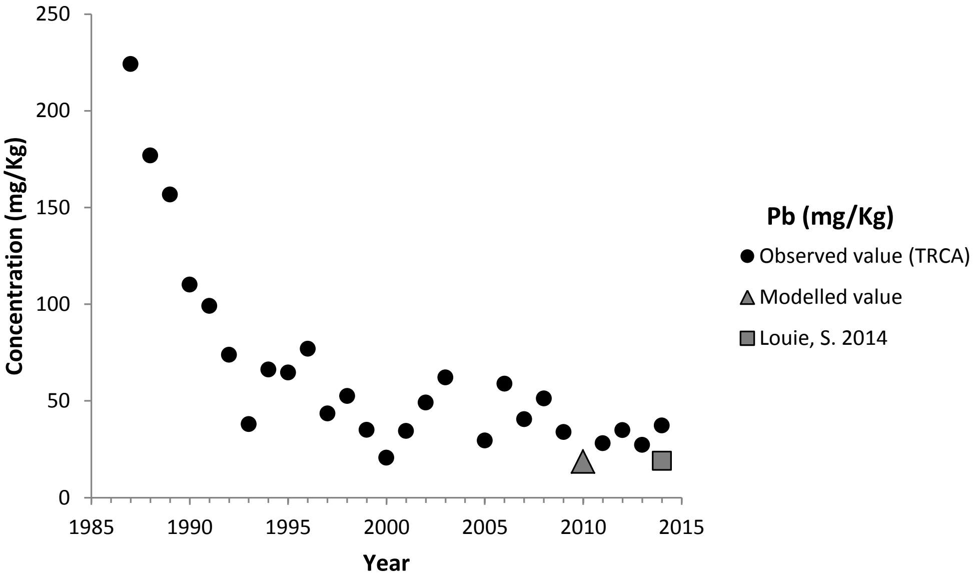

Figure 29: Lead concentration trend in the dredged sediment at Keating Channel. 1987 to 2014 data obtained from TRCA

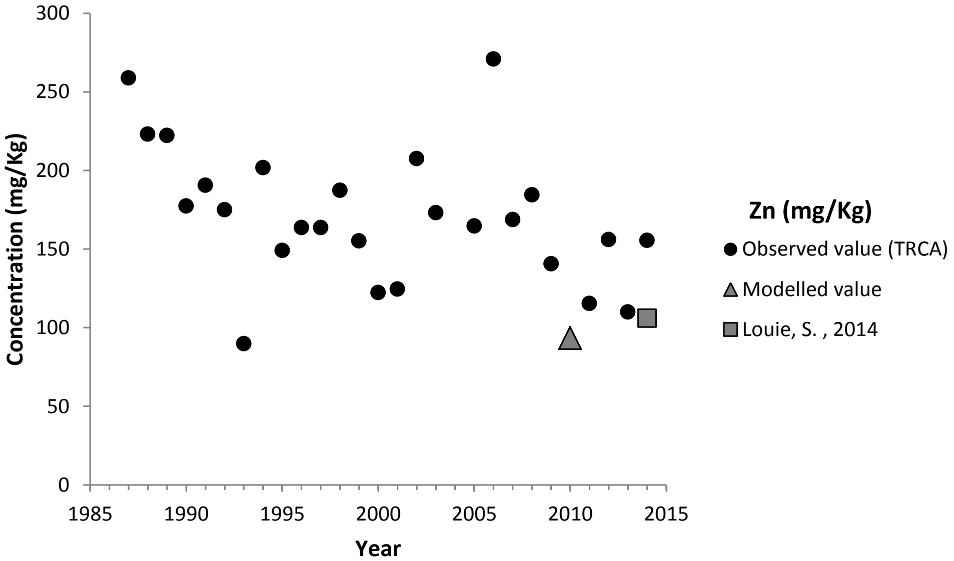

Figure 30: Zinc concentration trend in the dredged sediment at Keating Channel. 1987 to 2014 data obtained from TRCA

The spatial distribution of the sediment bed concentrations for each of the three metals, copper, lead, and zinc can be seen in Figure 31. The snapshots of model domain reported in the figure are at the end of the simulation period when the sediment bed metal concentrations are assumed to be in equilibrium. It can be observed that metal concentrations are relatively higher in sediment bed at two locations which can be termed as deposition hot spots. These deposition hot spot locations are at the mouth of the study reach where it enters into the Keating Channel and at north of the Todmorden monitoring site. These deposition patterns are justified by the fact that the bed slope at these locations is relatively shallow compared to the rest of the domain. Shallow bed slope can cause lower flow velocities compared to the critical value causing deposition of sediments and associated metals. Figure 10 provides the longitudinal profile of the study reach which confirms the relatively shallow bed slope regions at these locations. Therefore, the sediment bed metal distribution is considered representative of the natural conditions as a result of this analysis.

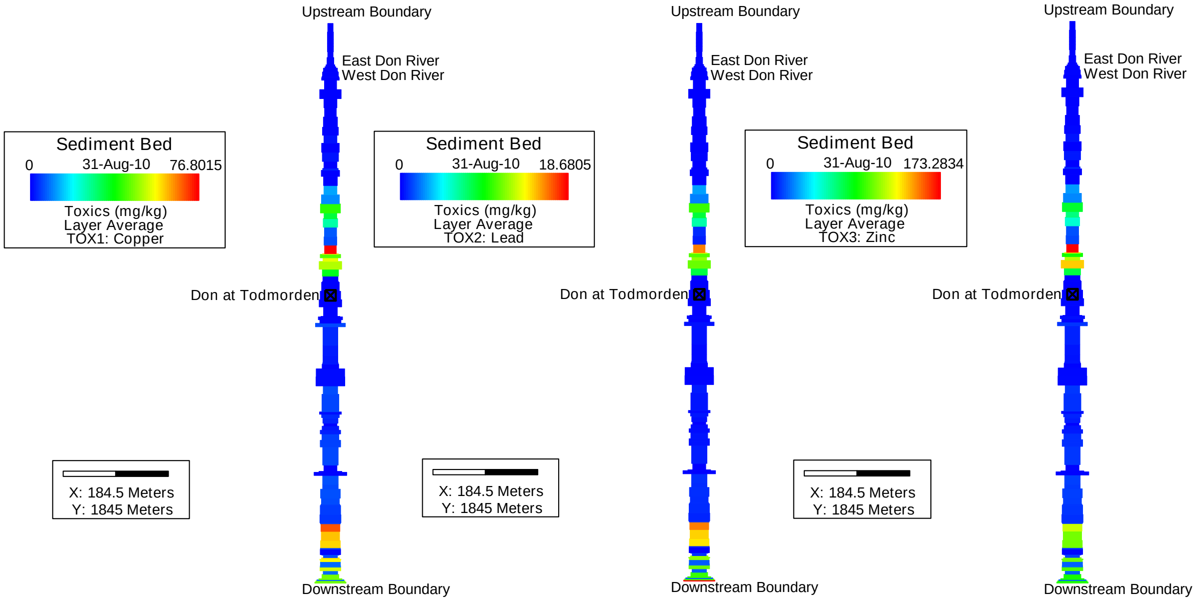

Figure 31: Spatial sediment bed concentration distribution for copper, lead, and zinc (left to right) at the end of simulation. Mapped using EFDC Explorer 7.2

The total bed sediments and bed metal loadings were also estimated at the end of the model simulation period at the mouth of the river. The total sediment mass was estimated to be 46.6 Kg/m^2 at the end of the model time period. This estimated sediment mass is multiplied with the sediment bed concentrations for copper, lead, and zinc to obtain total bed metal loadings at the mouth of the river.

These metal loadings are shown in Figure 32 using a GIS map of the study reach for illustrative purposes. The loadings are estimated to be 2177 mg/m^2 for copper, 872 mg/m^2 for lead, and 4350 mg/m^2 for zinc. These loadings show general consistency with the overall results for each metal, with zinc being the most abundant deposited metal at the mouth. However, no data is available for comparing these values to the observed bed masses. These loadings may be used to get the estimates of total sediments for dredging requirements at the river mouth, and which may also be useful in designing restoration plans.

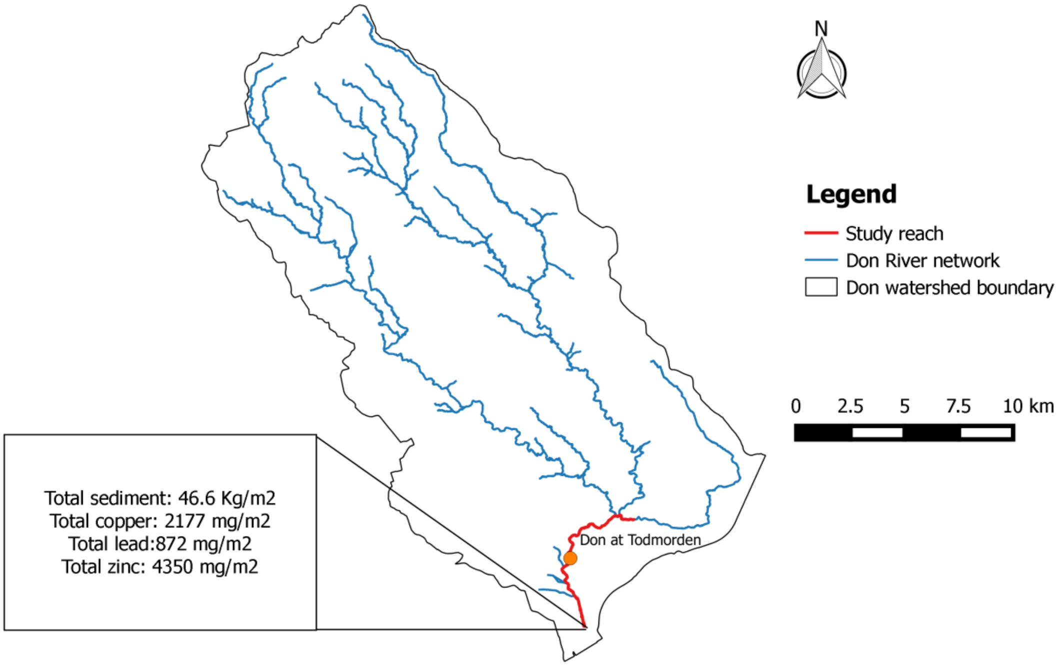

Figure 32: Total sediment and metals accumulation at the mouth of the river modelled by EFDC at the end of simulation. Mapped using QGIS 2.6

Chapter 6

Conclusions and Recommendations

The Don River watershed faces significant environmental challenges due to rapid urbanization and the associated flooding, erosion, and degrading water quality issues. This research, focused on the sediments and metals dynamics in the lower Don River, provides a representative model of the system. This model can be used as a predictive tool to estimate sediment and metal loads from the lower Don River to make informed management decisions.

The integration of the EFDC hydrodynamic model and the PCSWMM hydrologic model was successful using the STEMS tool. STEMS provided efficient setup of the EFDC model based on the results of the PCSWMM model. STEMS tool can be used on any river network modelled in PCSWMM that requires advanced analysis on sediment and pollutant transport using EFDC.

The hydrologic model for the Don River watershed developed by TRCA for a 40 day simulation from June 20, to July 30, 2008 was validated using a longer time span extending from April1 to August 31, 2010. The hydrologic results for flow at the Todmorden monitoring station were in good agreement with the observed data. Furthermore, it is concluded that the flow boundary conditions provided by the PCSWMM model control the hydraulic results of the EFDC model. The hydraulic results from PCSWMM and EFDC model show high correlation. This further elaborates the high sensitivity of EFDC hydraulic results to the flow boundary conditions provided by PCSWMM.

The sediments and trace metal transport is accurately represented by the EFDC model using the sediment and pollutant load boundary conditions from PCSWMM. The comparison between the sediments and metal results of the two models shows the importance of in-stream physical processes of a river. EFDC simulates the sediment transport processes including erosion, resuspension, and deposition for various size classes of sediments. Moreover, associated metals are simulated representing the proper sorption and diffusion mechanism. PCSWMM only simulates the sediment and pollutant loads from the subcatchments and routes them through the network using plug flow assumption. Although the same boundary loads are used for the two models, the difference in the spatial and temporal distribution of sediments and metals is significant. Therefore, EFDC results are used to represent the actual in-stream conditions while PCSWMM results are deemed reliable for providing the boundary loads to EFDC.

The modelled relationship between total sediment/pollutant concentrations and river discharge complements the observed data set at the Todmorden monitoring station. Therefore, it further provides verification of the EFDC model for sediment and metals transport simulation. It also suggests that most of the sediment and metals are transported in relatively shorter bursts within longer flood durations, further justifying the need of high frequency monitoring and modeling of sediment and metals transport in an urban river system.

The sediment bed metal distribution provides reasonable estimates of metal loads leaving the Don River system into the Keating Channel. Sediment bed metal concentrations are estimated to be 47.0 mg/Kg for copper, 10.4 mg/Kg for lead. The results are complementing the observed concentration data trend from the dredged sediments of the Keating Channel provided by TRCA. The results also complement the sediment bed concentrations from the research of (Louie, 2014). The sediment bed mass was estimated to be 46.6Kg/m^2, which provided bed metal concentrations of 2177mg/m^2 for copper, 872mg/m^2 for lead, and 4350mg/m^2 for zinc. The spatial trend in the sediment bed concentration show higher values at the relatively shallower bed slope locations further enforcing the reliability of the model. Therefore, the EFDC sediment and metals transport model is deemed a reliable predicting tool to estimate metal loads discharging into the Keating Channel through the deposited sediments, and their spatial distribution in the channel.

Several recommendations are suggested to further improve the model. The pollutant loads from PCSWMM are based on buildup/wash-off model for TSS using parameters relevant to similar sites. It is recommended that site specific parameters be used for accurate representation of the wash-off loads from the subcatchments. Further calibration of the PCSWMM model can be achieved through computational resources which can improve the boundary loads for EFDC model.

It is recommended that reliable precipitation data be made available for the entire year to increase the model time span to capture the snow melt period. PCSWMM model can then be upgraded to simulate snowmelt. Results of the model from this time period can be useful in assessing the quality of snowmelt and its impacts on the sediments and metals dynamics in the system.

Calibration of the EFDC model can be improved if high resolution monitoring data for the TSS and metal concentration in the Don River is available. However, it is understood that such high resolution monitoring may not be feasible due to limited resources. Therefore, it is recommended that a long term transport model based on a yearly scale be developed for better calibration of the EFDC model. Monthly monitoring data for TSS and metals concentration can provide extensive data set over several years for detailed calibration. However, such a long term continuous model requires reliable long term precipitation data as identified earlier and may also require a coarser spatial discretization for efficient results.

Appendix A

Miscellaneous Data

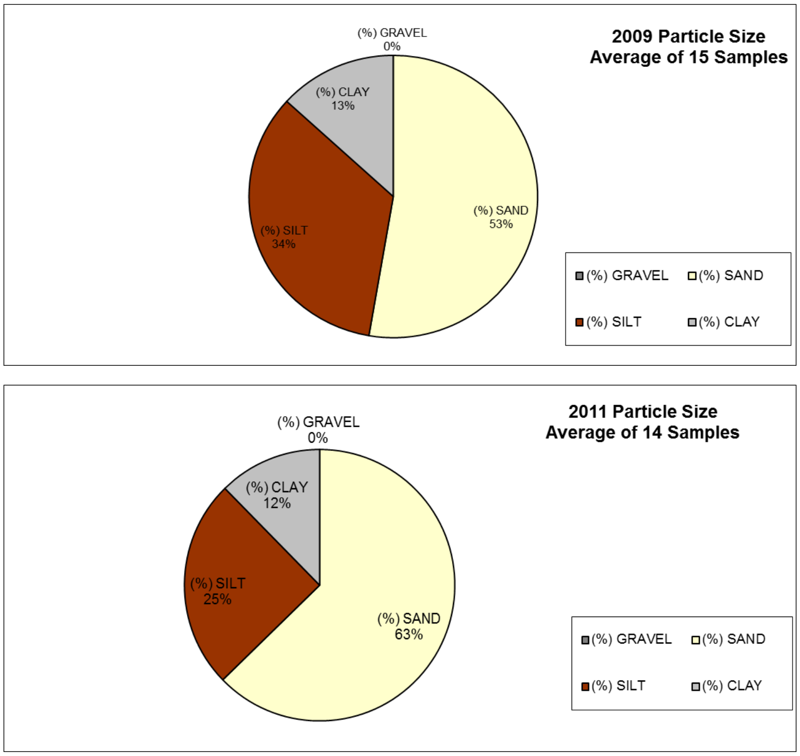

Figure A 1: Particle size distribution of the dredged sediments from the Keating Channel. Data courtesy of TRCA

Table A 1: Weighted porosity calculation for the sediment bed in EFDC. Classification of sediment bed based on dredged sediment particle size distribution provided by TRCA

Size Class	% Particle Size	Diameter (EFDC) (µm)	ASTM Classification	Reported porosity range (Geotechdata.info, 2013)	Used porosity
SAND	63	410	SP-SM	0.23 - 0.49	0.4
SILT	25	30	SM	0.25 - 0.49	0.4
CLAY	12	10	CH	0.39 - 0.59	0.5
				Weighted porosity for EFDC	**0.44**

Bibliography

Allison, J. D., & Allison, T. L. (2005). *Partition coefficients for metals in surface water, soil, and waste.* (No. EPA/600/R-05/074). Washington: U.S. Environmental Protection Agency.

Bai, Y., & Duan, J. G. (2014). Simulating unsteady flow and sediment transport in vegetated channel network. *Journal of Hydrology, 515*, 90-102. doi:10.1016/j.jhydrol.2014.04.030

Bicknell, B. R., Imhoff, J. C., Kittle, J. L.,Jr., Donigian, A. S., Jr., & Johanson, R. C. (1997). *Hydrological simulation program-Fortran, user's manual for version 11.* (No. EPA/600/R-97/080). Athens, Ga: U.S. Environmental Protection Agency, National Exposure Research Laboratory.

Bussi, G., Francés, F., Montoya, J. J., & Julien, P. Y. (2014). Distributed sediment yield modelling: Importance of initial sediment conditions. *Environmental Modelling and Software, 58*, 58-70. doi:10.1016/j.envsoft.2014.04.010

Cera, T. (2013). Swmmtoolbox 0.5.5. Retrieved from https://pypi.python.org/pypi/swmmtoolbox

Chen, C., Tsai, C., & Tsai, C. (2006). Simulation of sediment yield from watershed by physiographic soil erosion-deposition model. *Journal of Hydrology, 327*(3-4), 293-303. doi:10.1016/j.jhydrol.2005.11.031

Chen, C., Tsai, C., & Tsai, C. (2011). Simulation of runoff and suspended sediment transport rate in a basin with multiple watersheds. *Water Resources Management, 25*(3), 793-816. doi:10.1007/s11269-010-9727-4

Chu, X., & Rediske, R. (2012). Modeling metal and sediment transport in a stream-wetland system. *Journal of Environmental Engineering, 138*(2), 152-163.

City of Toronto. (2006). *Wet weather flow management guidelines*. City of Toronto.

Craig, P., M. (2015). *User manual for EFDC_Explorer 7.2: A pre/post processor for the environmental fluid dynamics code (Rev00).* (). Edmonds: Dynamic Solutions-International, LLC.

Deltares System. (2012). Sobek suite. Retrieved from http://www.deltaressystems.com/hydro/product/108282/sobek-suite

Deltares Systems. (2012). Delft3D suite. Retrieved from http://www.deltaressystems.com/hydro/product/621497/delft3d-suite

DHI. (2015). MIKE 11, river modelling unlimited. Retrieved from http://www.mikepoweredbydhi.com/products/mike-11

Ding, X., Shen, Z., Hong, Q., Yang, Z., Wu, X., & Liu, R. (2010). Development and test of the export coefficient model in the upper reach of the Yangtze River. *Journal of Hydrology, 383*(3–4), 233-244. doi:http://dx.doi.org/10.1016/j.jhydrol.2009.12.039

Ecosystems Research, E. (2013a). One dimensional riverine hydrodynamic and water quality model. Retrieved from http://www.epa.gov/athens/wwqtsc/html/epd-riv1.html

Ecosystems Research, E. (2013b). Water quality analysis simulation program (WASP). Retrieved from http://www.epa.gov/athens/wwqtsc/html/wasp.html

Geotechdata.info. (2013). Soil porosity. Retrieved from http://www.geotechdata.info/parameter/soil-porosity.html

Guo, Y., & Jia, H. (2012). An approach to calculating allowable watershed pollutant loads. *Frontiers of Environmental Science & Engineering, 6*(5), 658-671. doi:10.1007/s11783-012-0446-3

Hamrick, J. M. (1992). A three-dimensional environmental fluid dynamics computer code: Theoretical and computational aspects. *The College of William and Mary, Virginia Institute of Marine Science*, (Special Paper 317), 63.

Hossain, I., Imteaz, M., Gato-Trinidad, S., & Shanableh, A. (2010). Development of a catchment water quality model for continuous simulations of pollutants build-up and wash-off. *World Academy of Science, Engineering and Technology, 37*, 941-948.

Hu, J., Li, S., & Geng, B. (2011). Modeling the mass flux budgets of water and suspended sediments for the river network and estuary in the Pearl River Delta, China. *Journal of Marine Systems, 88*(2), 252-266. doi:10.1016/j.jmarsys.2011.05.002

Huang, W., Liu, X., & Chen, X. (2008). Numerical modeling of hydrodynamics and salinity transport in Little Manatee River. *Journal of Coastal Research*, 13-24. doi:10.2112/1551-5036-52.sp1.13

IRIC Project. (2010). IRIC software. Retrieved from http://i-ric.org/en/introduction

James, W. (2002). *Rules for responsible modeling* (3rd ed.). Guelph: CHI.

James, W., Rossman, L. E., & James, W. R. C. (2010). *Water system models - user's guide to SWMM 5* (13th ed.). Guelph: CHI Press Publication R242.

Ji, Z., Hamrick, J., & Pagenkopf, J. (2002). Sediment and metals modeling in shallow river. *Journal of Environmental Engineering-ASCE, 128*(2), 105-119. doi:10.1061/(ASCE)0733-9372(2002)128:2(105)

Ji, Z. (2008). *Hydrodynamics and water quality : Modeling rivers, lakes, and estuaries*. Hoboken, NJ: Wiley-Interscience.

Jia, H., Wang, S., Wei, M., & Zhang, Y. (2011). Scenario analysis of water pollution control in the typical peri-urban river using a coupled hydrodynamic-water quality model. *Frontiers of Environmental Science & Engineering in China, 5*(2), 255-265. doi:10.1007/s11783-010-0279-x

Jia, Y. (2012). *Technical manual of CCHE2D.* (No. NCCHE-TR-02-2013). Mississippi: National Center for Computational Hydroscience and Engineering.

Johnes, P. J. (1996). Evaluation and management of the impact of land use change on the nitrogen and phosphorus load delivered to surface waters: The export coefficient modelling approach. *Journal of Hydrology, 183*(3-4), 323-349. doi:10.1016/0022-1694(95)02951-6

Julien, P. Y. (2002). *River mechanics*. Cambridge; New York: Cambridge University Press.

Louie, S. (2014). *Metal loads in an urban stream catchment (Don River, Ontario).* (Unpublished MASc.). University of Waterloo, Waterloo.

Nash, J. E., & Sutcliffe, J. V. (1970). River flow forecasting through conceptual models part I - a discussion of principles. *Journal of Hydrology, 10*(3), 282-290.

Nelson, J.,M. (2010). *FaSTMECH solver manual*. Colorado: IRIC.

TRCA. (2009). *Don River watershed plan - beyond forty steps*. Toronto: Toronto and Region Conservation Authority.

TRCA. (2015a). DMNP EA receives provincial approval - January 28, 2015. Retrieved from http://www.trca.on.ca/the-living-city/green-infrastructure-projects/environmental-assessment-projects/don-mouth-naturalization-and-port-lands-flood-protection-project/whats-new.dot

TRCA. (2015b). Don River watershed. Retrieved from http://trca.on.ca/the-living-city/watersheds/don-river/

Trento, A., & Alvarez, A. (2011). A numerical model for the transport of chromium and fine sediments. *Environmental Modeling & Assessment, 16*(6), 551-564. doi:10.1007/s10666-011-9263-5

United Nations Statistics Division. (2015). UN data - A world of information. Retrieved from https://data.un.org/CountryProfile.aspx?crName=CANADA

USACE. (2010). *HEC-RAS river analysis system.* (No. CPD-68). Davis: US Army Corps of Engineers, Hydrologic Engineering Center.

Wang, C., Shen, C., Wang, P., Qian, J., Hou, J., & Liu, J. (2013). Modeling of sediment and heavy metal transport in Taihu Lake, China. *Journal of Hydrodynamics, 25*(3), 379-387. doi:http://dx.doi.org.proxy.lib.uwaterloo.ca/10.1016/S1001-6058(11)60376-5

Wu, W. (2008). *Computational river dynamics*. London; New York: Taylor & Francis.

Yu, S., Wu, Q., Li, Q., Gao, J., Lin, Q., Ma, J., Qiufang, X., & Wu, S. (2014). Anthropogenic land uses elevate metal levels in stream water in an urbanizing watershed. *Science of the Total Environment, 488-489* doi:10.1016/j.scitotenv.2014.04.061

Zhang, Y. (2005). *CCHE2D-GUI – graphical user interface for the CCHE2D model user's manual – version 2.2* . (No. NCCHE-TR-2005-03). Mississippi: Natonal Center for Computational Hydroscience and Engineering.

Zhang, Y., & Aral, M. M. (2004). Solute transport in open-channel networks in unsteady flow regime. *Environmental Fluid Mechanics, 4*(3), 225-247. doi:10.1023/B:EFMC.0000024237.17777.b1

Zhang, W., Jia, Q., & Chen, X. (2014). Numerical simulation of flow and suspended sediment transport in the distributary channel networks. *Journal of Applied Mathematics, 2014* doi:10.1155/2014/948731;